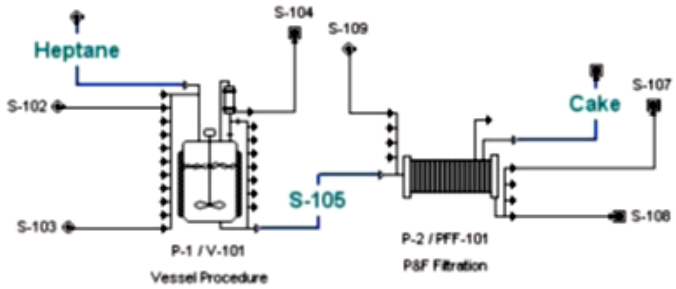
Case study :
Reaction /Filtration



DEVELOPING A PROCESS MODEL

The first example of this chapter demonstrates the key initialization and analysis steps for modeling a process with SuperPro Designer. The fundamental steps and analysis features used in this example are the same as the steps and features that would be used during the creation of any other type of process. Therefore, regardless of which type of process you intend to model, reading through the following example should provide you with the knowledge required to model processes on your own. In addition, since this example is a batch process, it serves as a medium for discussing several scheduling issues.

The following files are available for this example in the 'Examples\Misc' directory of SuperPro Designer:

1. *GettingStarted8_0a*: This file represents a simple batch process consisting of a reaction step (Batch Vessel Procedure in a Reactor) and a filtration step (Plate and Frame Filtration Procedure). The mass and energy balances for this process model are solved in equipment 'Design Mode' in order to determine equipment sizing parameters. The development and solution of this process model are described in sections 2.1b Starting a New Process File up to 2.1i Simulating the Process and Viewing the Simulation Results. Furthermore, the specification and analysis of scheduling, equipment utilization and resource tracking

information for this process model is described in sections 2.1j Setting the Process Scheduling Information up to 2.1k Viewing Scheduling, Equipment Utilization and Resource Tracking Results.

2. *GettingStarted8_0b*: This file is based on the previous one. The mass and energy balances are now solved for known equipment sizes in equipment 'Rating Mode' in order to analyze throughput and economic information. A throughput and debottlenecking analysis for this process is described in section 2.1l Throughput Analysis and Debottlenecking. Furthermore, the specification and analysis of economic information is described in section 2.1m Cost Analysis and Economic Evaluation.

For continuous processes, the steps that are related to scheduling of operations within unit procedures (see 2.1h Initializing Unit Procedures) and of the entire process (see 2.1j Setting the Process Scheduling Information) do not need to be performed.

2.1a Summary Steps

The steps listed below summarize the process of developing a process model with SuperPro Designer. These steps are explained in much greater detail in the remainder of this section.

1. Start a new process file by selecting option 'Start a New Process File' in the opening dialog of the program. Alternatively, you may start a new process file later by clicking **New** () on the **Main** toolbar or on the **File** menu of the program.
2. Initialize the process model using the following items of the **Tasks** menu: (a) set the plant operation mode (batch or continuous) using item **Set Mode of Operation**, (b) register pure components using item **Pure Components ▸ Register, Edit/View Properties** and stock mixtures using item **Stock Mixtures ▸ Register, Edit/View Properties**, and (c) if the plant operation mode is batch, specify recipe scheduling information using item **Recipe Scheduling Information**. You may also want to change the default physical units of the process model using item **Process Options ▸ Physical Units Options** on the **Edit** menu.
3. Build the process flowsheet by adding unit procedures from the **Unit Procedures** menu while in **Select Mode** (). Switch to **Connect Mode** () to draw streams and connect the unit procedures.
4. Add operations, such as Charge, Agitation, Batch Heating, Batch Stoichiometric Reaction, etc., to unit procedures. Different unit procedures have different operations available to them. Batch/semi-continuous (cyclical) unit procedures can contain one or more operations, whereas continuous unit procedures are equivalent to unit operations. After the desired operations have been added, initialize all operations and streams.
5. Complete the analysis of the process model using the following commands: (a) solve mass and energy balances and size equipment by clicking **Solve M&E Balances** ( ) on the the **Main** toolbar or on the **Tasks** menu, (b) classify streams into different categories (e.g., raw material, revenue, waste, etc.) using item **Stream Classification** on the **Tasks** menu, and (c) perform costing and economic evaluation calculations by clicking **Perform Economic Calculations** ( ) on the **Main** toolbar or on the **Tasks** menu. Other analyses related to scheduling, throughput and debotttlenecking may be optionally performed.

6. Generate charts and view analysis results using items of the **Tasks**, **Charts** and **View** menus. Generate and view reports using items of the **Reports** menu.

2.1b Starting a New Process File

To open SuperPro Designer after it has been installed, select the program shortcut on the Windows **Start** Menu or double-click the file 'Designer.exe' in the installation directory of the application. The following dialog box will appear by default:

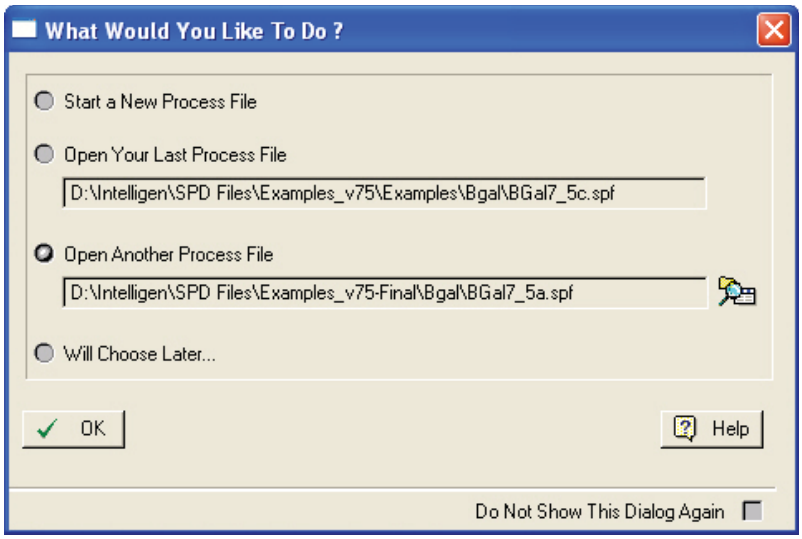


Figure 2.1: The opening dialog box of the program.

To begin working on a new process file, select the option named 'Start a New Process File' from the above dialog and click **OK**. If you select another option and close this dialog, you can always start a new process file later by clicking **New** ( ) on the **Main** toolbar on the **File** menu.

2.1c Specifying the Mode of Operation for the Entire Plant

After you choose to start a new process file, the 'Process Operating Mode' dialog box will appear as shown in Figure 2.2. This dialog box allows you to set the primary mode of operation (batch or continuous) and the annual operating time available for the entire process. You can also modify these settings at a later time by clicking **Set Mode of Operation** on the **Tasks** menu.

When the process operating mode is set to 'Batch', all stream flows are displayed on a per-batch basis. On the other hand, when the process operating mode is set to 'Continuous', all stream flows are displayed on a per-hour basis. Moreover, no scheduling information is necessary for plants operating continuously.

Please note that although the plant operation mode can be either batch or continuous, SuperPro Designer can also model processes that operate in mixed modes. That is, you can have continuous unit procedures in a batch process plant as well as batch/semi-continuous (cyclical) unit procedures in a continuous process plant. This is explained later in this chapter (see 2.1h Initializing Unit Procedures).

For now, let's select 'Batch' as the operating mode of this example process.

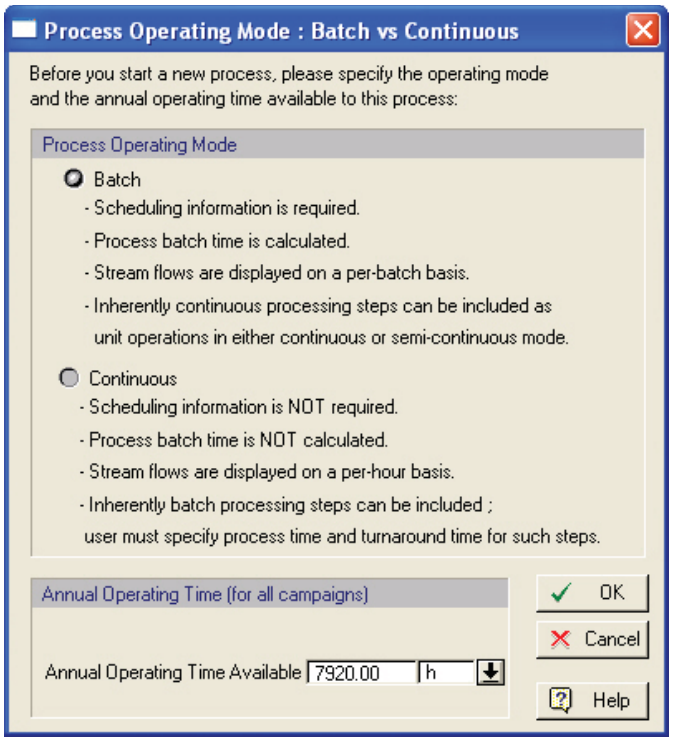

Process Operating Mode : Batch vs Continuous
Before you start a new process, please specify the operating mode
and the annual operating time available to this process:
Process Operating Mode
Batch
- Scheduling information is required.
- Process batch time is calculated.
- Stream flows are displayed on a per-batch basis.
- Inherently continuous processing steps can be included as
unit operations in either continuous or semi-continuous mode.
Continuous
- Scheduling information is NOT required.
- Process batch time is NOT calculated.
- Stream flows are displayed on a per-hour basis.
- Inherently batch processing steps can be included ;
user must specify process time and turnaround time for such steps.
Annual Operating Time (for all campaigns)
Annual Operating Time Available
7920.00
h
OK
Cancel
Help

Figure 2.2: The 'Process Operating Mode' dialog box.

2.1d Setting the Default Physical Units

SuperPro Designer provides a variety of options for units of measure for the entry and display of data. To view or modify the default units of the process model, click on an empty area in the flowsheet and select **Process options ▸ Physical Units Options** on the **Edit** menu. Alternatively, right-click on the flowsheet to bring up its context menu and select **Physical Units Options**.

*To activate the **Process Options** menu item on the **Edit** menu, you must first click on an empty area of the flowsheet.*

2.1e Registering Components and Mixtures

COMPONENT DATABANKS

SuperPro Designer provides for the use of multiple component databanks. The following component databanks can be used:

- the 'Designer' databank,
- the 'User' databank, and
- the DIPPR databank.

Each databank is contained in a separate database file. The ‘Designer’ databank is part of the ‘Designer’ (or ‘System’) database. It provides data for over 530 commonly used compounds.

The ‘User’ databank is part of the ‘User’ database an it is a repository available for users to store data for their own (or ‘user-defined’) components. The ‘User’ component databank, is originally (upon installation of the software) empty.

The DIPPR databank draws its data from the relational form of the DIPPR database. This component database has been developed and maintained at Brigham Young University. A demo version of the DIPPR databank with only 5 components is shipped with SuperPro Designer.

To change the location of the database files where each of the above databanks is stored, click **Availability, Passwords and Locations** on the **Databanks** menu to display the ‘Databases: Availability, Passwords and Locations’ dialog. For example, if the full DIPPR databank is available or if you want to use a different user database file that somebody else created, you must specify its location through that dialog; for more details, see 15.1 Database Registration.

REGISTERING COMPONENTS

All the components that will be used in a process model must be registered first. To register components (in other words, to make them available in your process model), select **Pure Components ▸ Register, Edit/View Properties** on the **Tasks** menu. This will activate the dialog shown below.

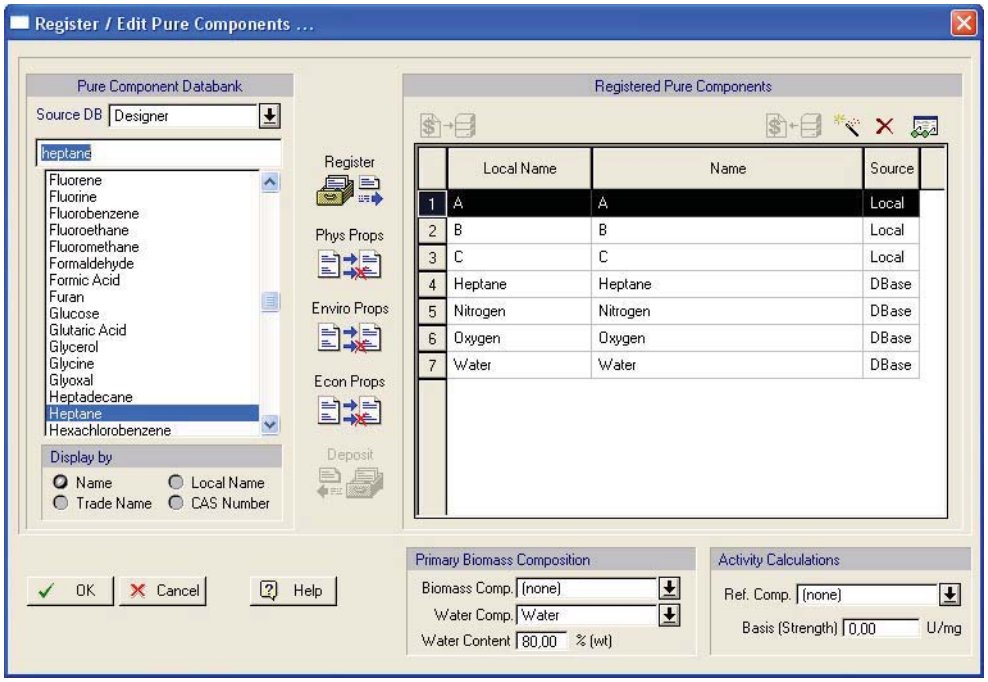


Figure 2.3: The pure component registration dialog box.

Note that pure components ‘Nitrogen’, ‘Oxygen’, and ‘Water’ are registered by default in every new process model and cannot be deleted. For this example process, you will need to add

'Heptane' to the list of registered pure components (shown on the RHS of this dialog) as well. To add 'Heptane', you can either scroll down to it in the list of available pure components in the 'Designer' database (shown on the LHS of this dialog), or you can begin typing "heptane" in the box above the list (see Figure 2.3) and the database will automatically scroll to the correct location. Next, click **Register** ( ) to add 'Heptane' to the list of registered pure components for this process model. Alternatively, you may double click on 'Heptane' in the database listing and it will be added to your list of registered components.

If a component is not available in the existing component libraries, you can click **New** ( ) on the 'Registered Pure Components' toolbar to create a new component for your process model. This will be automatically added to the list of registered components. For this process, you will need to create components 'A', 'B', and 'C'. These components will represent the reactants and products of a simple reaction. To create component 'A', click **New** ( ) and in the 'New Component Definition' dialog that appears (see Figure 2.4) fill-in the letter "A" for the 'Name' field. Notice that as you type, the contents of the 'Name' field are automatically copied to all other fields ('CAS Number', 'Trade Name', 'Local Name', 'Formula', and 'Company ID').

As far as the program is concerned, you do not need to have correct CAS Numbers, Formulas, etc. You just need to have something written in each of these six fields. The 'Local Name' is the one that appears in the reports and all the input/output dialog windows of the program.

Notice that at the bottom of this dialog, you can choose to initialize the properties of the new component by copying them from some other database component or registered component. For this example, click **OK** to copy the properties of component 'Water' which is available in the 'Designer' database to component 'A'.

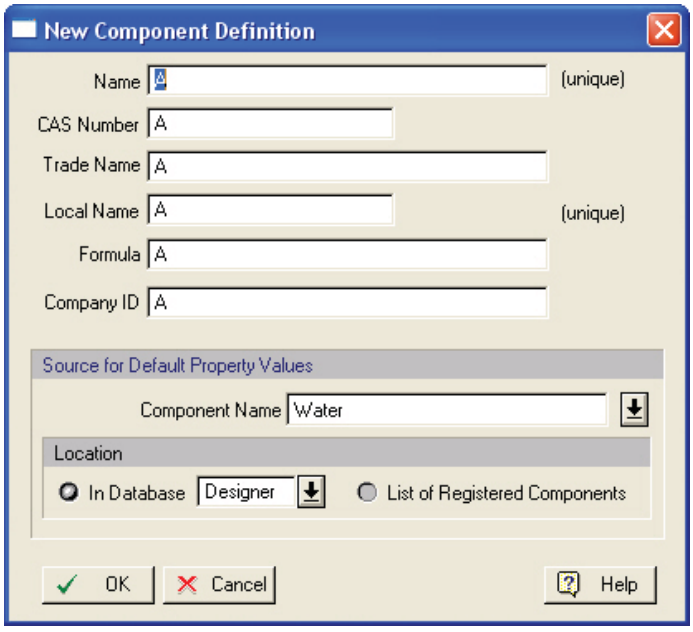


Figure 2.4: The 'New Component Definition' dialog box.

After you have added component 'A' to your list of registered components, follow the same steps to add components 'B' and 'C'. When you have completed this, you should edit some of

the properties of these components. To access the properties of component ‘A’, double-click on the component in the list of registered pure components. Alternatively, you can highlight the component (by clicking on it) and then click **Properties** ( ) on the ‘Registered Pure Components’ toolbar. This will bring up the ‘Pure Component Properties’ dialog box for component ‘A’. Through this dialog you can view or edit a component’s physical and environmental properties, cost data, and regulatory information.

For the purposes of this example, the only physical parameter we will be concerned with is the molecular weight (MW). Please go to the ‘Physical (Constant)’ tab and change the MW of component ‘A’ to 150 g/gmol as shown in Figure 2.5. Also, visit the ‘Economics’ tab and specify a purchasing price of $10/kg. Then, click **OK** to close the dialog.

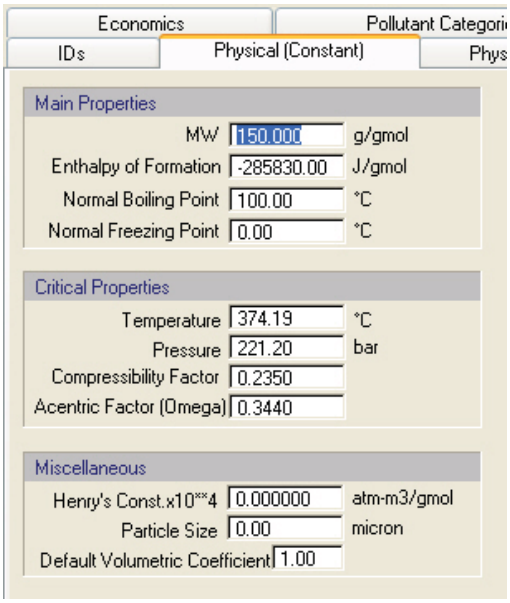


Figure 2.5: Editing the constant physical properties of component ‘A’ in the example.

Next, please visit the properties dialog for component ‘B’ and enter a MW of 25 g/gmol and a purchasing price of $15/kg. Also, visit the properties dialog for component ‘C’ and enter a MW of 175 g/gmol and a selling price of $300/kg. This completes your initialization of components for our simple example.

To delete a registered pure component, highlight that component in the list of registered pure components and click ***Delete*** *( ) on the ‘Registered Pure Components’ toolbar.*

You can add registered pure components, which you have created or modified, to the ‘User’ databank, so that you can register these components in other files as well. To add a component to the ‘User’ databank, first select the databank in the ‘Source DB’ drop-down list. Then, highlight a registered component and click on the ***Deposit*** *button:*

The current version of SuperPro Designer does not make use of the Normal Freezing Point of pure components. The corresponding field entry, which can be found in the 'Physical (Constant)' tab of the 'Pure Component Properties' dialog, can be ignored.

REGISTERING MIXTURES

Mixtures are used to facilitate initialization of input streams in cases where certain raw materials (e.g., buffers) are consumed as mixtures. In order to register a mixture, click Stock Mixtures } Register, Edit/View Properties on the Tasks menu and follow the same steps as for registering pure components.

2.1f Saving and Opening Files

At this point, please save your file by clicking **Save As** from the **File** menu and giving your process model a descriptive name in the Windows 'Save As' dialog box that appears. In general, it is a good idea to save your work often in order to avoid having to redo work in the event of a program crash.

When working with larger process files, include the date or some other version indicator in the saved case name.

If the program does crash, there is sometimes a possibility that you will not be able to re-open the file you were most recently working on. In that case, you should try to open the backup versions of your file. Anytime you save a newer version of your file, SuperPro Designer will also save a backup copy of the previous version using file extension '.sp~' (as opposed to a normal '.spf' file). If the '.sp~' backup file already exists, SuperPro Designer will first create a copy of that file using file extension '.s~~' as a second backup.

To open a file, click **Open** from the **File** menu. This will bring up the Windows 'Open' dialog box. To open a backup file, simply go to the directory where you saved your original file, select the corresponding '.sp~' or '.s~~' backup file (select 'All Files (*.*)' in the 'File Type' field of the dialog box) and click the **Open** button.

Note that the corresponding file extensions for the original, backup, and second backup files in EnviroPro Designer are '.epf', '.ep~' and '.e~~'.

2.1g Building the Process Flowsheet

ADDING UNIT PROCEDURES

The first step in building a flowsheet is to add processing steps (unit procedures) to the process. A unit procedure is defined as a series of operations that take place within a piece of equipment. The types of operations available depend on the type of unit procedure you are using. As explained later in this chapter (see 2.1h Initializing Unit Procedures), batch/semi-continuous (cyclical) unit procedures can contain one or more operations, whereas continuous unit procedures are equivalent to unit operations.

To add a unit procedure to the flowsheet, first select the desired unit procedure from the **Unit Procedures** menu. For our example, please select **Batch Vessel Procedure ▸ in a Reactor**. Notice that after you select a unit procedure and move the mouse pointer to the flowsheet area, it changes to the 'add step' pointer (add step). This indicates that your next mouse

click on the flowsheet will lay down the icon of the selected unit procedure in that location. Please click near the left side of the flowsheet to lay down the icon of the selected unit procedure. SuperPro Designer automatically adds a default procedure name ('P-1'), host equipment name ('V-101') and procedure description ('Vessel Procedure') below the icon.

After you have added a Batch Vessel Procedure in a Reactor to the flowsheet, please add a Plate and Frame Filtration Procedure by clicking **Filtration ▸ Plate and Frame Filtration** on the **Unit Procedures** menu and then clicking somewhere to the right of the vessel procedure icon. Your flowsheet should now look something like this:

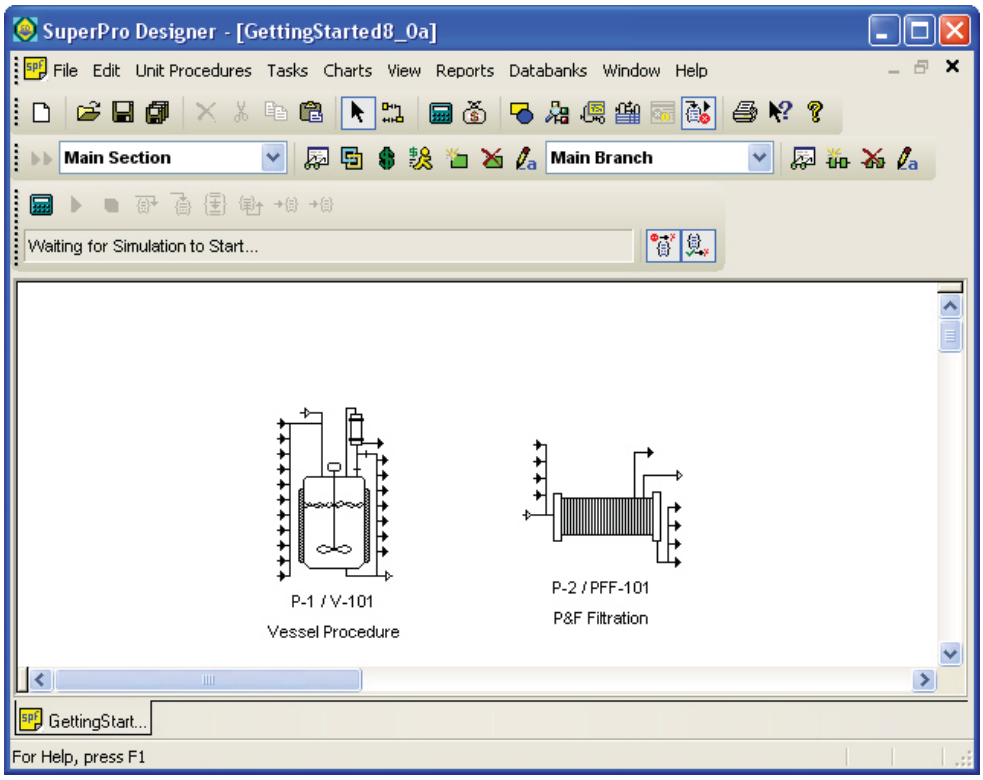


Figure 2.6: The example process with the Batch Vessel Procedure in a Reactor and Plate and Frame Filtration Procedure icons added.

*If you decide to abort the addition of the new unit procedure, you can simply hit the **Esc** key on your keyboard.*

*If you wish to modify the default equipment prefixes (e.g. 'V' for a Stirred Reactor (CSTR) vessel and 'PFF' for a Plate & Frame Filter), click **Application Settings** on the **File** menu and go to the 'Prefixes' tab. To edit the prefix of an equipment resource, highlight that equipment in the available list and click on the corresponding prefix. Through the same tab, you can also modify the default operation prefixes in the same manner; for more details, see 8.20 Application Settings.*

Moving, Copying and Deleting Unit Procedures

The following guidelines show how you can move or delete unit procedures in a flowsheet, and how you can cut or copy and paste unit procedures to a different location in the same flowsheet or in another flowsheet.

First, you need to select the desired unit procedure icon(s). You can select a single icon by clicking on it. You can select multiple icons by either dragging an enclosing rectangle around them, or by adding icons to the selection. To add an icon to the selection, click on it while holding down the **Ctrl** key. To remove an icon from the selection, **Ctrl+Click** on it again. To select an entire flowsheet, click **Select All** on the **File** menu or press **Ctrl+A**.

▶ To Move Unit Procedures...

1. Select the desired unit procedure icon(s).
2. Drag the selected icon(s) to the new location. If multiple icons are selected, you can drag any member of the selection and all icons will move simultaneously. You can use the arrow keys to move the selection one pixel at a time.

Note that when you move a unit procedure icon that has streams attached to it, all streams will move with it. If two unit procedures are connected through an intermediate stream and both the source and destination unit procedures move, then the stream will keep its structure intact and move with them. If one of the stream's ends remains anchored while the other end is being moved, then the stream will adjust its first and/or last elbow to accommodate the change of location; for more details on streams, see 'Adding Streams' on page 2-14.

▶ To Delete Unit Procedures...

1. Select the desired unit procedure icon(s).
2. Hit the **Delete** key on your keyboard or click **Clear** on the **Edit** menu. The selected unit procedure(s) will be erased.

When you delete a unit procedure, all streams attached to it will also be deleted.

▶ To Cut or Copy and Paste Unit Procedures...

SuperPro Designer allows you to cut or copy unit procedures into the clipboard so that you can subsequently paste them to a different location, either in the same flowsheet or in another flowsheet. To do this:

1. Select the desired unit procedure icon(s).
2. To cut the icon(s), click **Cut** on the **Edit** menu (or press **Ctrl+X**). To copy the icons, click **Copy** on the **Edit** menu (or press **Ctrl+C**).
3. Move the mouse cursor to the desired area in the same flowsheet or in another flowsheet and click **Paste** on the **Edit** menu (or press **Ctrl+V**) to paste the icon(s).

The following restrictions apply to the use of the Cut, Copy and Paste features:

1. You cannot cut or copy and paste streams alone. Streams are placed onto the clipboard only if you cut or copy multiple unit procedures.
2. When pasting unit procedures into a flowsheet, you should be aware that certain features of the original unit procedures are *not transferred* into the newly created copy:
   (a) When you cut or copy a single unit procedure, attached streams are not included in the pasted set.
   (b) If the start time of the first operation of the pasted unit procedure was defined on a relative basis (e.g., with respect to the start or end of another operation in some other procedure), then the scheduling of the pasted procedure is reset to remove the coupling.
   (c) If the original unit procedure was sharing equipment with another procedure, the pasted procedure is reset to be executed in its own equipment.
3. Pasting streams and certain processing steps with component- and stock mixture- related specifications from one flowsheet to another is not possible unless all components and stock mixtures of the source process model exist in the destination process model as well. If that is not the case, the program will automatically expand the set of registered pure components and stock mixtures in the destination process to include the missing ones.

If you want to paste icons into another application (e.g., a word processing application), please consult Chapter 14 (Exchanging Data with Other Apps).

Accessing the Help Files

In many equipment resources that host unit procedures, there are dedicated ports, such as 'Feed', 'Vent (Emissions)', 'Cake Removal', 'Filtrate Removal', etc. To see which ports are

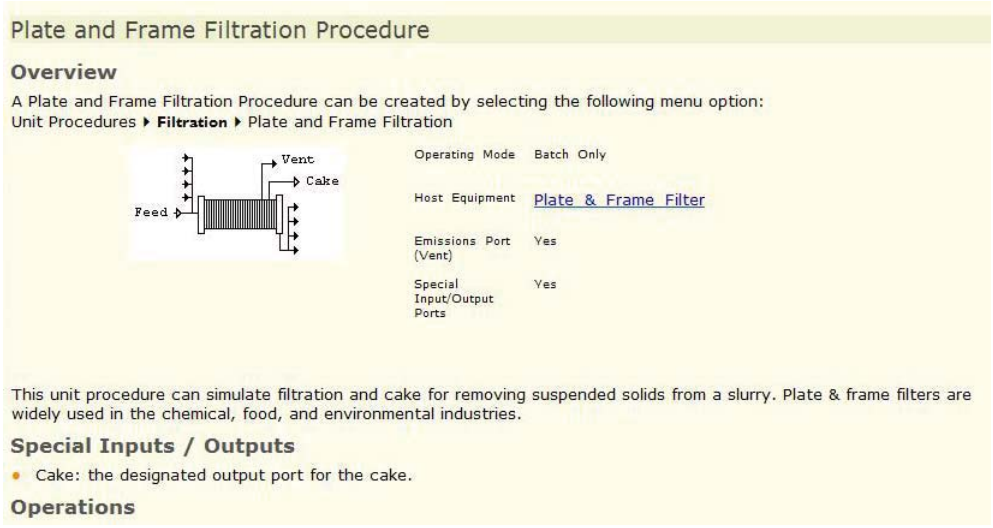


Plate and Frame Filtration Procedure
Overview
A Plate and Frame Filtration Procedure can be created by selecting the following menu option:
Unit Procedures ▸ Filtration ▸ Plate and Frame Filtration
Vent
Cake
Feed
Operating Mode
Batch Only
Host Equipment
Plate & Frame Filter
Emissions Port (Vent)
Yes
Special Input/Output Ports
Yes
This unit procedure can simulate filtration and cake for removing suspended solids from a slurry. Plate & frame filters are widely used in the chemical, food, and environmental industries.
Special Inputs / Outputs
Cake: the designated output port for the cake.
Operations

Figure 2.7: The help topic for the Plate and Frame Filtration Procedure.

dedicated to each function, you can look up the desired equipment or unit procedure in the program's Help system, which is available through the **Help** menu. This provides access to supporting documentation shipped with the software, such as the electronic version of the User's Manual and additional content.

As a shortcut to the **Help** menu for any unit procedure, you can click **Help** ( ) on the **Main** toolbar and then click on the unit procedure icon you are interested in. Alternatively, you can click on the unit procedure icon and hit the **F1** key. Note that you can also use the **Help** ( ) button feature as a shortcut to access the Help files for other interface elements, such as menu options, toolbar buttons, dialog boxes and dialog tabs.

At this point, please open the Help file for the Plate and Frame Filtration Procedure. A portion of that file is shown in Figure 2.7. Notice that dedicated ports of the host equipment (Plate & Frame Filter) are labeled next to its icon. The Help file for each unit procedure also contains a general description, links to its operation models and to the host equipment, and much more.

ADDING STREAMS

After you add a unit procedure to the process flowsheet, you can add streams. There are three types of streams:

- feed (input) streams,
- intermediate streams, and
- product (output) streams.

Feed streams do not have a source unit procedure and in batch processing they are mainly utilized by charge operations. Intermediate streams connect two unit procedures and they are used to transfer material from the source to the destination unit procedure. Product streams do not have a destination unit procedure. All streams are automatically identified with a stream tag.

In order to add streams to the flowsheet, you must first click **Connect Mode** ( ) on the **Main** toolbar. When you do this and return to the flowsheet, the mouse pointer changes to the 'add stream' pointer ( ) to indicate that you are in 'Connect Mode' (as opposed to 'Select Mode'). Then, you can add feed, intermediate, and product streams as described below:

▶ To Add a Feed Stream...

1. Click on an empty area in the flowsheet to initiate drawing of the stream. Notice that as you move the mouse pointer over the inlet and outlet ports, it changes to a 'port' pointer ( ).
2. Move the mouse pointer over the desired inlet port of the destination unit procedure and once the 'port' pointer is displayed click on the port to terminate the stream line. SuperPro Designer automatically draws the feed stream symbol at the beginning of the stream and labels the stream.

▶ To Add an Intermediate Stream...

1. Move the mouse pointer over the desired outlet port of the source unit procedure and once the 'port' pointer is displayed click on the port to initiate drawing of the stream.

2. Move the mouse pointer over the desired inlet port of the destination unit procedure and once the 'port' pointer is displayed click on the port to terminate the stream line. SuperPro Designer automatically labels the stream.

▶ To Add a Product Stream...

1. Move the mouse pointer over the desired outlet port of the source unit procedure and once the 'port' pointer is displayed click on the port to initiate drawing of the stream.
2. Double-click on an empty area of the flowsheet to terminate the stream. SuperPro Designer automatically draws the product stream and labels the stream.

Note that between initiation and termination of a stream, you may optionally click at intermediate points on the screen to create right angle bends. This permits customizing of the stream route and flexibility in flowsheet design. You can cancel the stream-drawing process at any time by simply hitting the Esc key on your keyboard. Then you can restart the stream-drawing process by clicking **Connect Mode** ( ) again on the **Main** toolbar. To delete a stream, simply hit the **Delete** key on your keyboard.

At this point, please add the feed, intermediate, and product streams to your example process. Your flowsheet should now look like what is shown in Figure 2.8:

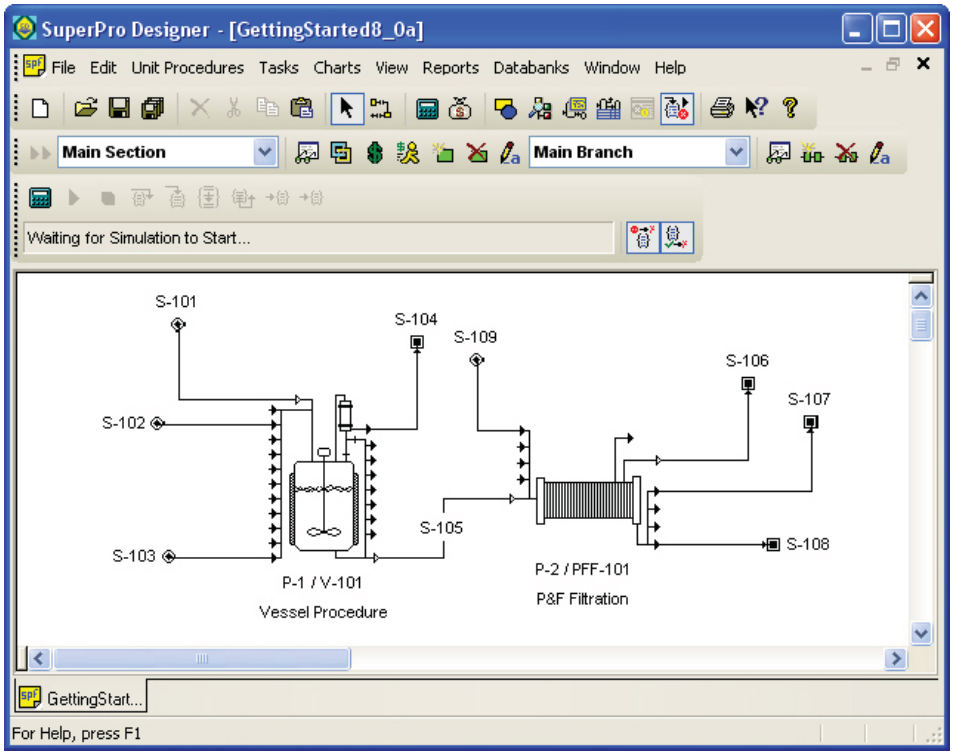


Figure 2.8: The example process flowsheet with streams added.

Changing the Appearance of Streams

When SuperPro Designer is in 'Select Mode' and the mouse pointer is over a stream line, it changes to a 'menu' pointer ( ) to indicate the availability of a stream context menu (see Figure 2.9). This menu can also be displayed by right-clicking on a stream line.

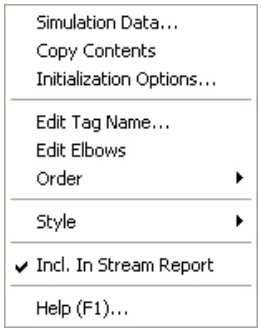


Figure 2.9: The stream context menu.

Through the stream context menu, you can view or edit (in case of input streams) the composition, flowrate, and other stream properties using item **Simulation Data**, select different stream initialization options using item **Initialization Options**, change the tag name (label) of the stream using item **Edit Tag Name**, adjust the elbows of the stream line using item **Edit Elbows**, edit the stream style (e.g., label and line color, line thickness, etc.) using item **Edit Style**, etc. Note that double-clicking on a stream line is equivalent to clicking **Simulation Data** on the stream's context menu.

At this point, please right-click on input stream 'S-101' of the vessel procedure 'P-1' and click **Edit Tag Name** on the stream's context menu. Change the name of the stream to 'Heptane' and click **OK**. Then, right-click on the 'Heptane' stream line and click **Style ▸ Edit Style** to display the 'Stream Style' dialog. In the 'Stream Line' tab (see Figure 2.10) of this dialog, click **Pen Color** ( ) on the 'Stream Line' toolbar and change the color to blue. Also click **Pen Size** ( ) on the same toolbar and change the size to 2 pixels.

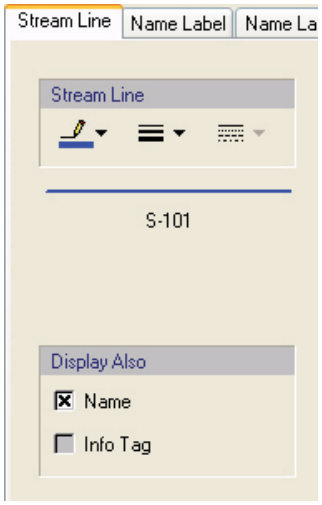


Figure 2.10: The 'Stream Line' tab of the 'Stream Style' dialog box.

Now, switch to the 'Name Label' tab. Click **Font Color** ( ) on the 'Color / Font' toolbar and change the color to teal. Also, click **Font** ( ) on the same toolbar and change the font style to bold and the font size to 12. Then, click the 'Name Label: Location' tab, change the segment preference to 'Vertical Near Source' and click **OK**.

Next, please change the name of stream 'S-106' (the stream that is connected to the dedicated cake removal port of the Plate & Frame Filter) to 'Cake'. Also, apply the style of the 'Heptane' stream to the 'Cake' stream and to the intermediate stream 'S-105' using the shortcut method described below:

▶ To Apply the Style of a Stream to Several Other Streams...

1. Right-click on the source stream line (e.g., the 'Heptane' stream in the example) and click **Style ▸ Pickup Style**.
2. Right-click on the desired target stream line(s) (e.g. the 'Cake' and 'S-105' streams in the example) and click **Style ▸ Apply Style**.

After applying these changes, your streams should look something like this:

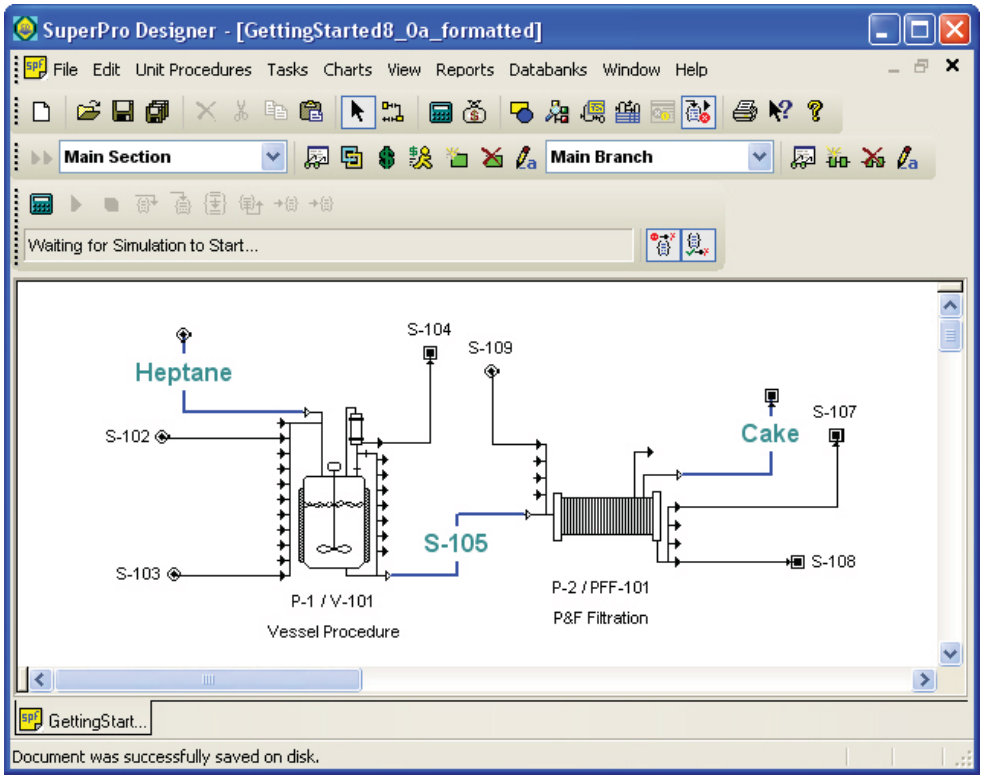


Figure 2.11: The example process flowsheet after the names and styles of streams have been changed.

For more information on stream drawing, see 4.10 Classification of Input and Output Streams.

2.1h Initializing Unit Procedures

SPECIFYING THE OPERATING MODE OF UNIT PROCEDURES

Each unit procedure added to the process has its own operating mode setting. This can be either:

- batch/semi-continuous, or
- continuous.

Batch/semi-continuous (cyclical) unit procedures can contain one or more operations, whereas continuous unit procedures are equivalent to unit operations. There are unit procedures that are inherently batch/semi-continuous (e.g., the Batch Vessel Procedure in a Reactor employed in this example) and can only be operated in batch/semi-continuous mode. You can have batch/semi-continuous unit procedures in continuous process plants. Other unit procedures are inherently continuous (e.g., the Centrifugal Pumping unit procedure which is available by clicking **Transport (near)** ▸ **Liquids** ▸ **Centrifugal Pump** on the **Unit Procedures** menu). By default, these can be operated in either mode. Thereby, you can have continuous unit procedures in batch process plants. Note that the operating mode of inherently continuous unit procedures is initially set to batch/semi-continuous in batch process plants and continuous in continuous process plants.

You can access or modify (where both options are available) the operating mode of a unit procedure through its context menu. Please right-click on a unit procedure icon bring up its context menu. The context menu of vessel procedure 'P-1' after operations are added in this example is shown in Figure 2.12. To view the operating mode setting of a unit procedure, click **Procedure Data**. This will display the 'Procedure Data' dialog for that unit procedure. The operating mode specifications can be found in the 'Scheduling' tab of that dialog; for more details on the operating mode of unit procedures, see Chapter 5 (Procedures & Operations).

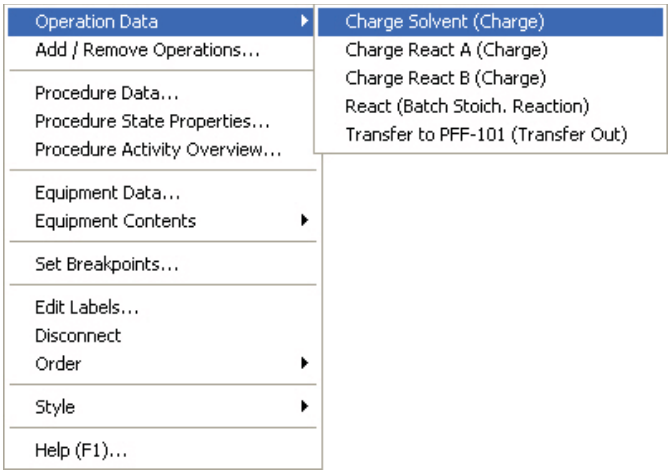


Figure 2.12: The context menu of the Batch Vessel Procedure in a Reactor in the example.

The meaning of each item in the context menu of a unit procedure is explained below:

- The **Operation Data** item allows you to access or modify the simulation parameters of the operations that have been added to the unit procedure. Note that this item is not

available if no operations have been added to the unit procedure. If the unit procedure contains a single operation, clicking on this menu item will bring up the 'Operation Data' dialog for that operation. If it contains more than one operations, clicking on this menu item or simply moving the mouse pointer over it will bring up a drop-down list of all added operations. Clicking on an operation in that list will bring up its 'Operation Data' dialog.

- The **Add/Remove Operations** item allows you to add/remove operations to/from the unit procedure and change the sequence in which these operations are executed. This item is only available for unit procedures that are operated in batch/semi-continuous mode.
- The **Procedure Data** item allows you to access or modify the simulation parameters of the unit procedure, such as the operating mode (continuous or batch/semi-continuous) and additional scheduling, throughput analysis and debottlenecking information.
- The **Procedure State Properties** item allows you to access or modify thermodynamic state properties of pure components during each operation.
- Through the **Procedure Activity Overview** item, you can view a summary of scheduled operations, processed material, and equipment contents during the execution of the unit procedure.
- The **Equipment Data** item allows you to access or modify the simulation parameters of the host equipment, such as sizing, costing, and scheduling information.
- The **Equipment Contents** item allows you to access or modify the initial equipment contents, and also view a summary of the thermodynamic properties and composition of the equipment contents during the execution of the unit procedure.
- The **Set Break Points** item allows you to place stops in the sequential solution of mass and energy balances. This is normally used for troubleshooting in large or complex process simulations.
- The **Edit Labels** item allows you to change the name of the unit procedure, the name of the host equipment and the description of the unit procedure. For example, you can change the default unit procedure name ('P-1'), equipment name ('V-101') and unit procedure description ('Vessel Procedure') for the vessel procedure in this example.
- The **Disconnect** item deletes all streams connected to the unit procedure.
- The **Flip (reverse flow direction)** item allows you to change the flow direction of the unit procedure icon from left-to-right (default) to right-to-left and vice versa. You can also do that by clicking **Flip Horizontally** ( ) on the **Visual Objects** Toolbar (see 13.5 Visual Objects Toolbar). Note that this option is only available when the unit procedure does not have any streams attached to it.
- The **Order** item forces the unit procedure icon to appear behind or in front of other icons, text, etc.

- The **Style** item allows the user to edit such things as the icon color, the tag name color and font, etc.
- The **Help (F1)** item provides access to the Help file of the unit procedure.

ADDING OPERATIONS TO UNIT PROCEDURES

The next step toward initialization of unit procedures is to add relevant operations to each unit procedure. This step is generally required for unit procedures that are operated in batch/semi-continuous mode. For convenience, some inherently batch/semi-continuous unit procedures may initially contain one or more operations when added to the process (e.g., the Plate and Frame Filtration Procedure used in this example initially has a Cloth Filtration operation). An equivalent operation is always added to unit procedures that are inherently continuous, when these are added to the process (e.g., the Centrifugal Pumping unit procedure will contain a Centrifugal Pumping operation).

In order to add operations to a unit procedure that is operated in batch/semi-continuous mode, you can either:

- double-click on a unit procedure icon, or
- right-click on the unit procedure icon and select **Add ▸ Remove Operations** from the context menu of that unit procedure. Note that this menu item is only available for unit procedures that are operated in batch/semi-continuous mode.

Either action will bring up the 'Operation Sequence' dialog (see Figure 2.13) for the selected unit procedure.

Double-clicking on a continuous unit procedure (e.g., a Centrifugal Pumping unit procedure added to a continuous process plant) brings up the dialog window of its operation instead of the 'Operation Sequence' dialog. Essentially, a unit procedure that is operated in continuous mode behaves like a single operation.

At this point, please open the 'Operation Sequence' dialog for the vessel procedure ('P-1') in the example. Add a Charge operation to the operation sequence for this unit procedure by double-clicking this item in the list of available operations. Alternatively, you can highlight this item and click **Add** ( ) to add the new operation at the end of the operation sequence or **Insert** ( ) to insert the new operation *before* the highlighted operation in the operation sequence. To delete an operation from the operation sequence, click **Delete** ( ) on the available toolbar. If you add an operation in the wrong order, you can change its position in the operation sequence using the **Move Up** ( ), **Move Down** ( ), **Move to Top** ( ), and **Move to Bottom** ( ) buttons on the same toolbar.

Notice that when the charge operation is initially named 'CHARGE-1' when it is added to the operation sequence. Double-click that item (or highlight that item and click **Rename** ( ) on the available toolbar) and change the name of the added charge operation to 'Charge Solvent'. Now, add two more Charge operations, a 'React (Stoichiometric)' (Batch Stoichiometric Reaction) operation, and a Transfer Out operation, to the operation sequence. Rename these operations to 'Charge React A', 'Charge React B', 'React' and 'Transfer to PFF-101',

respectively, so that your dialog box looks like the one shown in Figure 2.13. Then click **OK** to return to the process flowsheet.

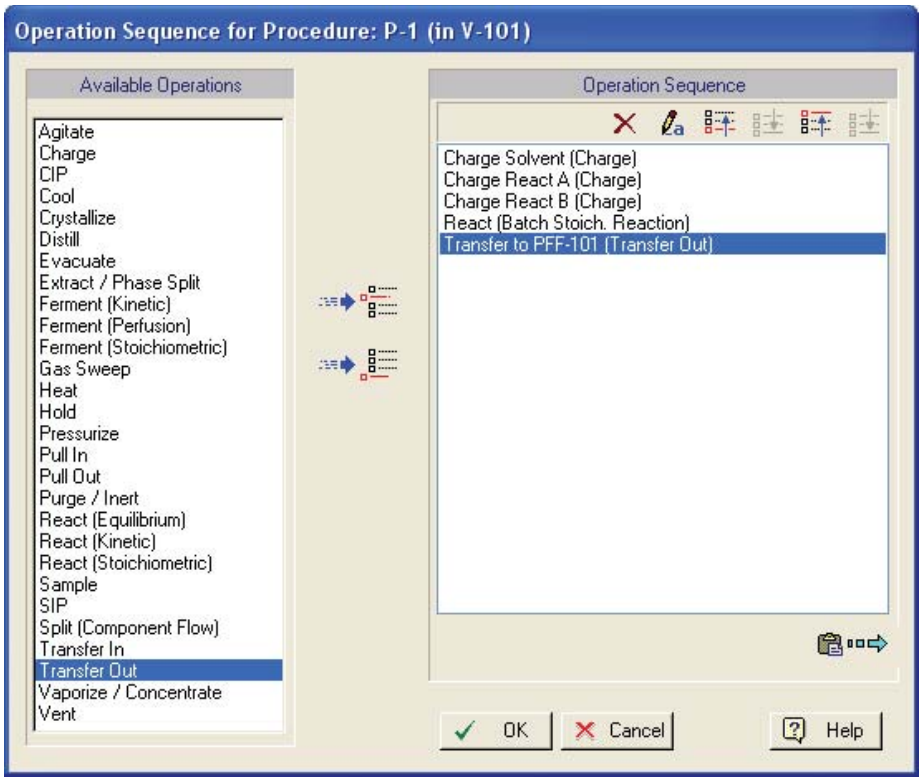


Figure 2.13: Adding operations to the Batch Vessel Procedure in a Reactor in the example.

Subsequently, please open the 'Operation Sequence' dialog for the filtration procedure ('P-2') in the example. Notice that this unit procedure has a 'Filter' (Cloth Filtration) operation (named 'FILTER-1') added to its operation sequence by default. Use the same method as before to add a 'Wash Cake' (Cake Wash) operation (named 'CAKE-WASH-1') and a Transfer Out operation (named 'TRANSFER-OUT-1') to the operation sequence. You can keep the default names for these operations.

INITIALIZING THE OPERATIONS

The next step is to initialize the operations added to the two unit procedures as described below.

Batch Vessel Procedure in a Reactor

Please right-click on the vessel procedure ('P-1') to bring up its context menu and click **Operation Data ▸ Charge Solvent (Charge)**. This will bring up the 'Operation Data' dialog for the 'Charge Solvent' operation. Through this dialog, you can access or modify the simulation data for an operation, such as the operating conditions, scheduling data, emission specifications, and labor-related information. This data is grouped into several tabs. Note that

different tabs may be available for different operations. The operating conditions (‘Oper. Cond’s’) tab for the ‘Charge Solvent’ operation of this example is shown in Figure 2.14.

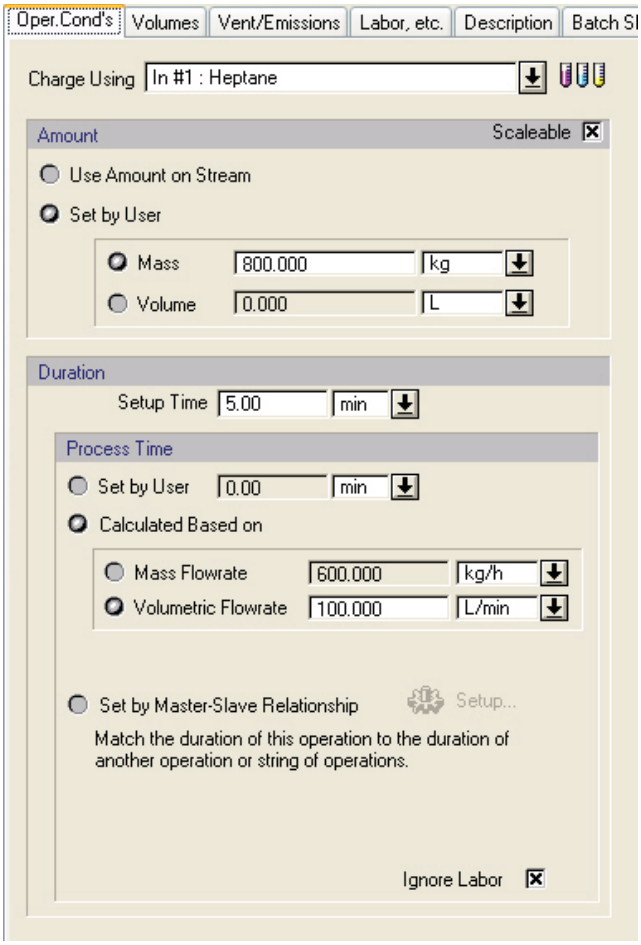


Figure 2.14: The ‘Oper. Cond’s’ tab for the first Charge operation (‘Charge Solvent’) in procedure ‘P-1’.

To initialize the operating conditions for the ‘Charge Solvent’ operation, you begin by selecting the charge stream for this operation. Use the ‘Charge Using’ drop-down list at the top of the tab to select the stream which you renamed ‘Heptane’ earlier in this section. Then, click on the **View/Edit Stream Composition and/or Amount** ( ) button next to the drop-down list in order to access the simulation data dialog for that stream (see Figure 2.15) and specify its

composition. To add ‘Heptane’ to the stream, double-click on the corresponding item in the ‘Registered Ingredients’ listing for that stream.

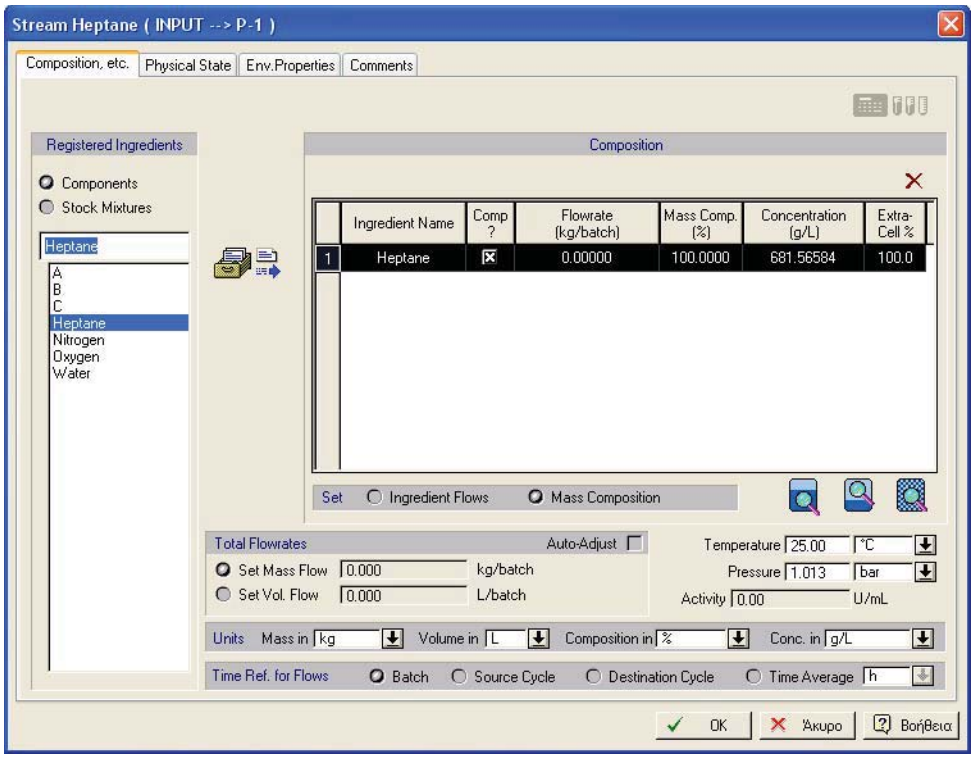


Figure 2.15: The simulation data dialog for the ‘Heptane’ stream.

Please note the following with respect to the simulation data dialog of streams:

1. You can charge multiple components in the same stream if you wish. To do this, simply add additional component names from the ‘Registered Ingredients’ listing. If the ‘Ingredient Flows’ option is selected, you can specify the corresponding amounts of added ingredients. The computer will automatically calculate the mass (%) and concentration (g/L or mole/L) of each ingredient, the stream’s density (if it is not set by the user), the volumetric flowrate and the activity of the stream. If the ‘Mass Composition’ option is selected, you can specify the total mass or volume flow and the mass (%) of each component. You may also select units for entry and display.
2. In addition to pure components, stock mixtures can be fed (or “charged”) into a process step using an input stream. To add a stock mixture to the stream, select the ‘Stock Mixtures’ option for registered ingredients and follow the same guidelines as for adding components.
3. As an alternative to going through the simulation data dialogs of operations to edit stream properties, you can initialize and edit input streams directly from the flowsheet itself. To do this, double-click on a stream (or right-click on a stream and click **Simulation Data** from the context menu of that stream). This will bring up the same dialog box as the one shown in Figure 2.15. Note that only the feed (input) streams to the flowsheet need to be specified.

The flowrates and compositions of intermediate and output streams are calculated by the program. However, the user can specify the physical state properties of these streams.

4. For biotech processes, the extracellular percentage ('Extra-Cell %') of an ingredient represents the fraction of that ingredient in the bulk solution (as opposed to inside the cell). For more information on this topic, please refer to the β-Galactosidase example (see 2.3 The b-Galactosidase Process).
5. If the plant operation mode is batch, all flowrates are reported on a per-batch basis (or per cycle of source or destination process step). If the process plant is set to operate in continuous mode, then all flowrates are reported on a per-hour basis. The choice for mass units can be made from each stream's dialog. This choice overwrites the default choices of physical units for the whole process as specified by selecting **Process Options ▸ Physical Units Options** on the **Edit** menu.
6. The 'Environmental Properties' tab of a stream's simulation data dialog displays the concentrations and daily throughputs of the environmental and aqueous properties of the stream (TOC, CaCO3, TP, TKN, COD, ThOD, BOD5, BODu, etc). All values are for display only and cannot be edited by the user through this dialog box. However, the environmental properties of the pure components contained in that stream (which contribute to the above stream properties) can be edited by selecting **Pure Components ▸ Register, Edit/View Properties** on the **Tasks** menu. To edit the environmental properties of a pure component, double-click on the desired component in the list of registered pure components and in the dialog that comes up click the 'Aqueous' tab.

For more details on streams and their properties, see Chapter 4 (Streams).

After you have specified the composition of the 'Heptane' stream, click **OK** to return to the operating conditions tab for the 'Charge Solvent' operation. Then, specify the amount of material that is going to be charged (800 kg). Notice that there are several ways that the duration of this operation can be specified. For this example, change the setup time of your charge to 5 minutes and set the volumetric flowrate to 100 L/min so that your tab looks like the one shown in Figure 2.14.

To enter a new value in different units than the ones selected you must first change the units prior to entering the new value.This is necessary since the units selection list acts as a unit converter, and changing the units will automatically convert the existing value to the selected units.

Please also visit the 'Volumes', 'Vent/Emissions', 'Labor etc', and 'Scheduling' tabs to see what they contain. A brief description of each of these tabs follows:

- 'Volumes' tab: Through this tab, the user can specify the maximum and minimum allowable working / vessel volume for this operation (i.e., by the end of the charge operation the vessel should not be more than 90 % full). In 'Design Mode' this is taken into account for sizing the equipment. In 'Rating Mode', the program makes sure that a vessel is not overfilled or the level does not drop below the agitator level.
- 'Vent/Emissions' tab: Through this tab, the user can specify which volatile organic compounds (VOCs) will be emitted, whether a sweep gas will be used (for emissions associated with reaction and crystallization operations), and what temperature the vent

condenser should be set at. SuperPro Designer is equipped with VOC emission models that are accepted by EPA. For more details, see Chapter 10 (Emissions).

- 'Labor, etc.' tab: Through this tab, the user can specify labor requirements and auxiliary utilities.
- 'Scheduling' tab: The is the right-most tab of all batch unit procedures. Through this tab, the user can specify the start time and duration for an operation. Note that no scheduling information is required for unit procedures that are operated in continuous mode.

Depending on the complexity of an operation, additional tabs may be used to display other pertinent variables.

For the heptane charge in your example process ('Charge Solvent'), please switch to the 'Vent/Emissions' tab and click the 'Venting' box and then the 'Emissions' box (see Figure 2.16). By default, the port that is connected to stream 'S-104' is selected as the venting port.

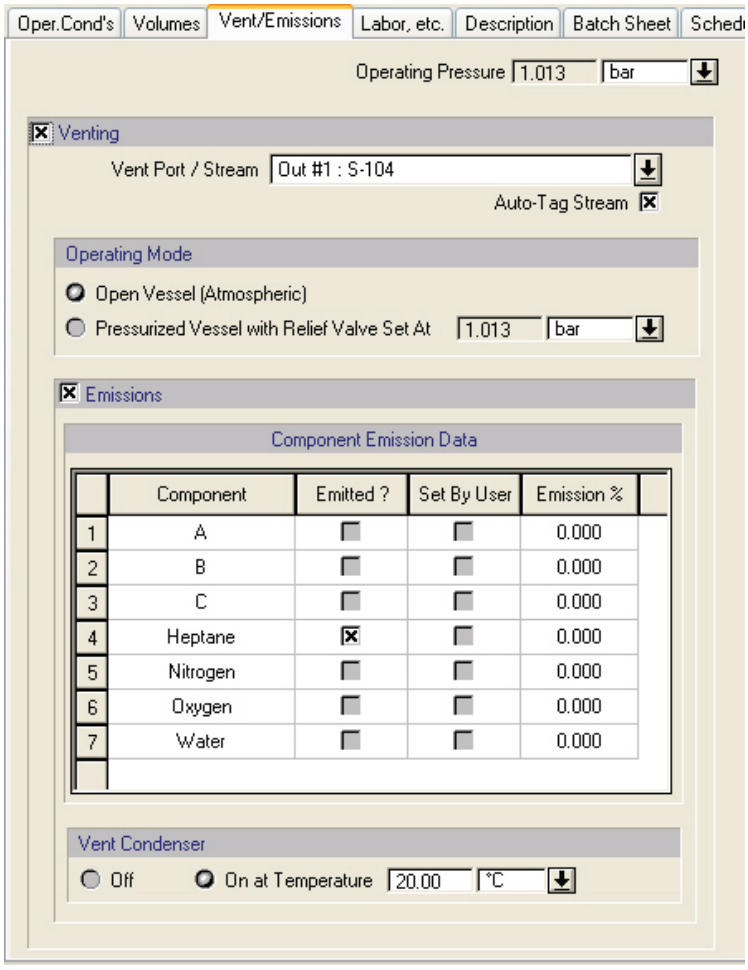


Figure 2.16: The 'Vent/Emissions' tab for the first Charge operation ('Charge Solvent') in procedure 'P-1'.

Then, check the ‘Emitted ?’ box next to the ‘Heptane’ component. After the simulation, please remember to visit the simulation data dialog of stream ‘S-104’ and check the amount of emitted ‘Heptane’. Note that for particulate and other components for which emission models are not available, the user can specify directly the emission percentage. For this operation, leave all the default values for the ‘Volumes’, ‘Labor, etc.’ and ‘Scheduling’ tabs.

Next, click **OK, Next Operation** (✔») on the simulation data dialog to move to the second Charge operation (named ‘Charge React A’) in this unit procedure. For this operation, use stream ‘S-102’ to add 50 kg of material ‘A’ to the reactor (please remember to visit the stream’s simulation data dialog and add material ‘A’ to the stream). Also specify a 5 minute setup time and a 20 kg/min charge rate. Keep the default values for the other tabs. Then, click **OK, Next Operation** again to move to the final Charge operation (named ‘Charge React B’). For this operation, use stream ‘S-103’ to add 40 kg of material ‘B’. Also change the setup time to 5 minutes and the charge rate to 20 kg/min.

Click **OK, Next Operation** once more to move to the Batch Stoichiometric Reaction operation (named ‘React’). Notice that the ‘Oper. Cond’s’ tab is different for this operation than it was for the charge operations. Also, two additional tabs are present. These include a ‘Fed Batch’ tab that contains available specification options for fed-batch supply of reactants, and a ‘Reactions’ tab (see Figure 2.17) in which reaction parameters are specified.

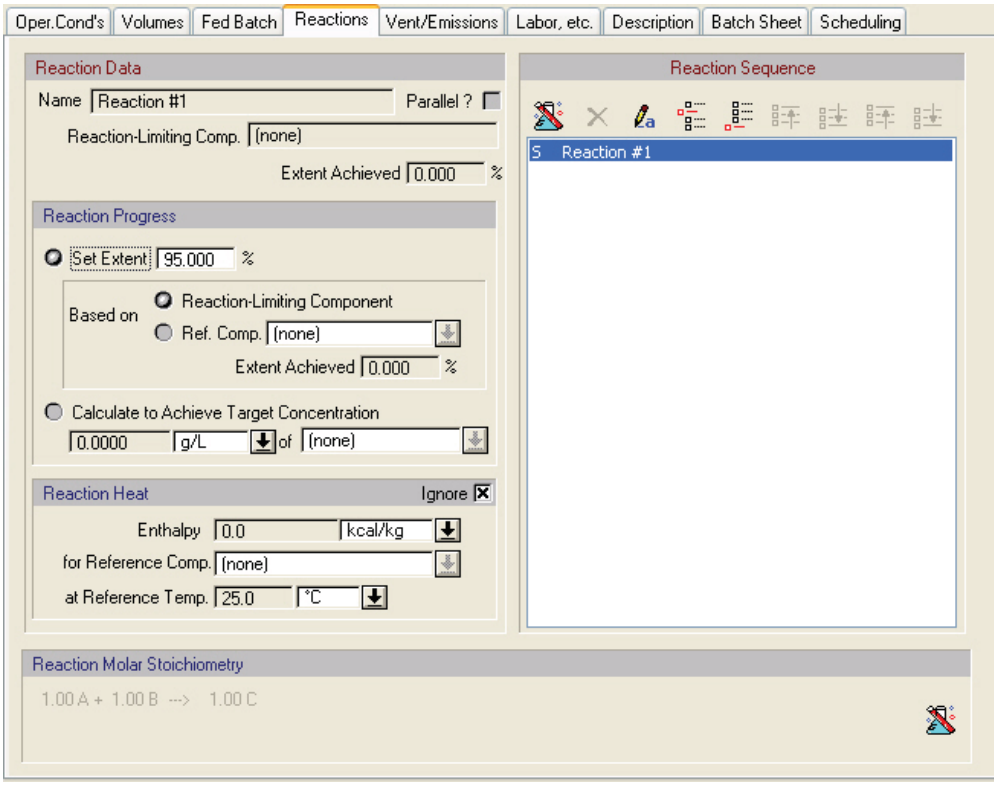


Figure 2.17: The ‘Reactions’ tab for Batch Stoichiometric Reaction operation ‘React’ in procedure ‘P-1’.

Starting with the operating conditions tab, please change the final temperature to 50 ^{o}C and the process time to 6 hours. Also, select ‘Steam’ as the heat transfer agent by clicking the ‘Agent’

drop-down list box and double-clicking ‘Steam’ on the ‘Heat Transfer Agents’ drop-down listing that is available in the right pane. Keep the default values of all other parameters in this tab. Next, referring to the ‘Volumes’ tab, notice that you can specify a maximum and minimum working-to-vessel volume ratio. Change the ‘Max Allowable Working/Vessel Volume’ to 80%. Then, move to the ‘Reactions’ tab (see Figure 2.17).

In this tab, you will need to specify the parameters describing a reaction in which a molecule of reagent (A) combines with a molecule of reagent (B) to form a molecule of product (C):

$$A + B \rightarrow C$$

To enter this, click **Edit Stoichiometry** ( ) to bring up the ‘Stoichiometry Balance’ dialog for Reaction #1 (see Figure 2.18). Introduce the reactants (pure components ‘A’ and ‘B’) and the product (pure component ‘C’) using the **Add a Reactant** and **Add a Product** toolbar buttons (located above the reactant and product tables, respectively). Select the ‘Molar’ option for the specification of the stoichiometric coefficients and keep the default unit molar coefficient for everything; for more details on specifying the stoichiometry balance for a reaction, see 2.2d Initialization of Reaction Operations. Now, click **OK** to close this dialog and return to the ‘Reactions’ tab.

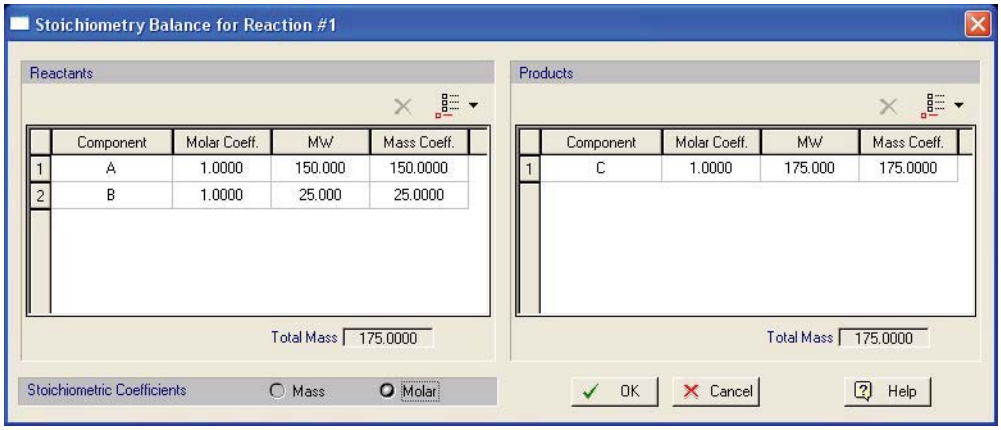


Figure 2.18: The ‘Stoichiometry Balance’ dialog box for the example reaction.

In addition to specifying the stoichiometric reaction coefficients, you will need to specify the extent of the reaction. For this example, set the extent to 95%, as was done in Figure 2.17.

Leave all the default values for the ‘Vent/Emissions’, ‘Labor. etc.’, and ‘Scheduling’ tabs and click **OK, Next Operation** to move to the ‘Operation Data’ dialog for the Transfer Out operation (‘Transfer to PFF-101’). In the operating conditions tab (see Figure 2.19), use the drop-down menu at the top of the screen to specify which stream will be used for the transfer operation (stream ‘S-105’ is the only choice for this example). In addition, in order to accurately capture the time required for this operation, set the duration to be the same as the duration of the filtration operation in procedure ‘P-2’. To do that, select the ‘Set By Master-Slave Relationship’ duration option and then click the **Setup** button. Through the dialog that comes up, select ‘P2 (in PFF-101)’ as the Master Procedure (through the ‘Another Procedure’ drop-down list), ‘FILTER-1 (Cloth Filtration)’ as the Master Operation (through the ‘Match a Single Operation’ drop-down list) and then click **OK**. This will ensure that the reactor will be

considered “utilized” during filtration, since the reactor will not be completely emptied until the filtration is complete. You can leave the default values for the other tabs in this dialog. Click **OK** to return to the flowsheet.

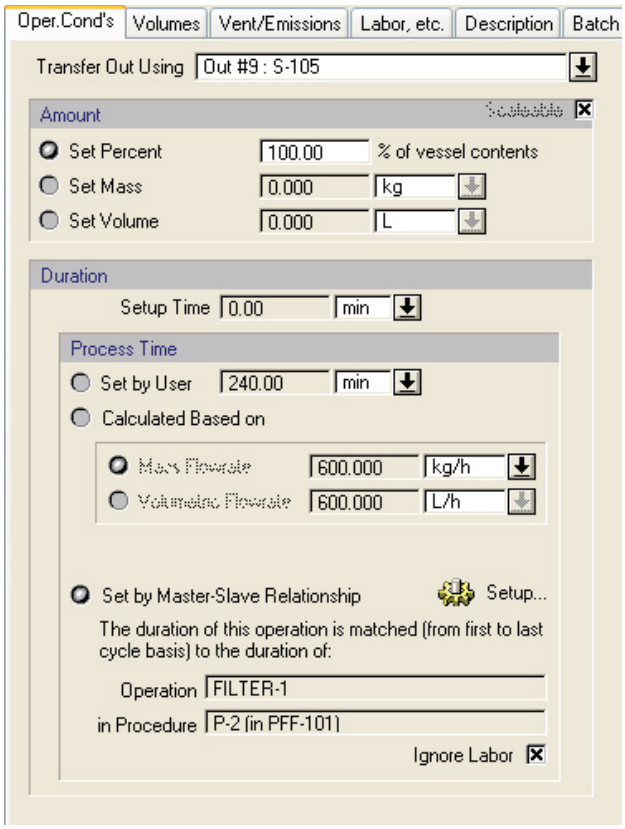


Figure 2.19: The ‘Oper. Cond’s’ tab for Transfer Out operation ‘Transfer to PFF-101’in procedure ‘P-1’.

Plate and Frame Filtration Procedure

Next, you will need to initialize the operations in the filtration procedure (‘P-2’). Please right-click on unit procedure ‘P-2’ and select **Operation Data ▸ FILTER-1 (Cloth Filtration)** from the context menu of that unit procedure. This will bring up the ‘Operation Data’ dialog for the Cloth Filtration operation (named ‘FILTER-1’).

The operating conditions tab for this operation is shown in Figure 2.20. For the purposes of this example, let us assume that reagents ‘A’ and ‘B’ are completely soluble in ‘Heptane’, whereas the product ‘C’ is virtually insoluble in ‘Heptane’. In the ‘Particulate Component Removal’ table that is available on the top left corner of this tab, please specify that 95% of your product ‘C’ will be removed from the feed stream and will remain on your filter, whereas the rest will end up in the filtrate. Also notice that you can specify a cake dryness either based on loss on drying (LOD) or cake porosity. This value will cause a portion of the ‘Heptane’ solvent and of soluble components ‘A’ and ‘B’ to be held in your wet cake. Please change the LOD for your filtration to 35%. By specifying a LOD of 35%, you are telling the program that only 65% of wet cake is the insoluble product C. For this operation, please specify a filtration time of 3

hours. Keep the rest of the parameters (such as the filtrate flux of 200 L/m^2-h) as they are and also, keep stream 'S-107' as the filtrate stream.

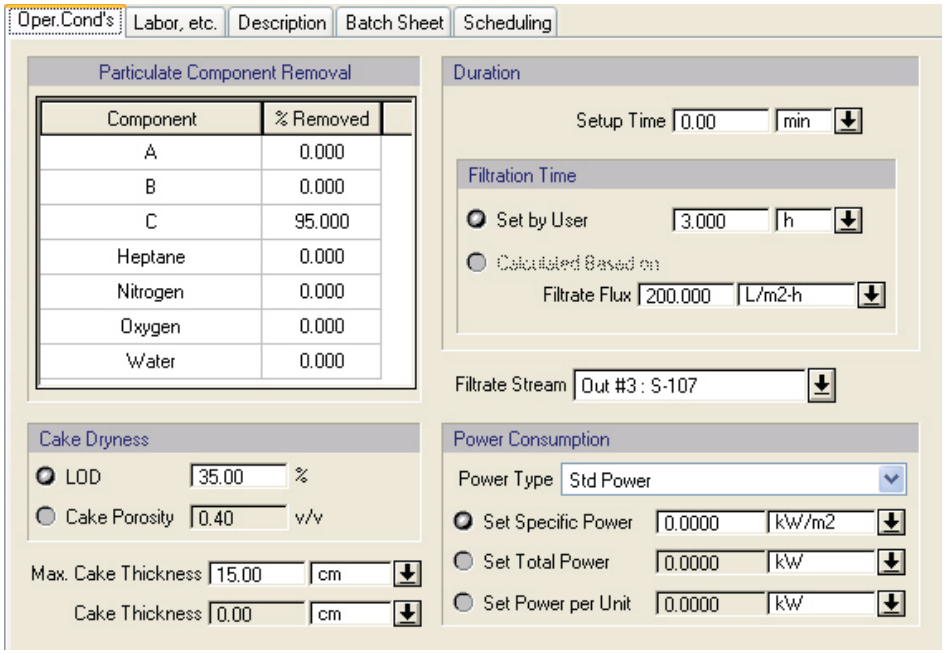


Figure 2.20: The 'Oper. Cond's' tab for Cloth Filtration operation 'FILTER-1'in procedure 'P-2'.

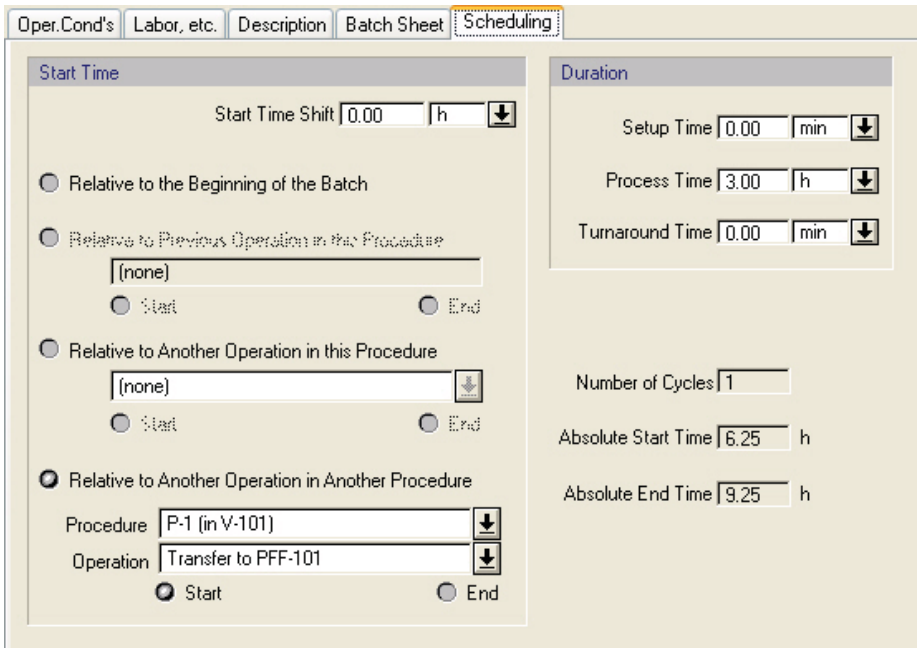


Figure 2.21: The 'Scheduling' tab for Cloth Filtration operation 'FILTER-1'in procedure 'P-2'.

Next, please visit the ‘Scheduling’ tab of the filtration operation. This tab is common to all operations in batch unit procedures. By default, the first operation in any batch unit procedure is scheduled to start relative to the beginning of the batch. In order to accurately schedule your filtration, you will need to change the start time to be relative to the start of the Transfer Out operation ‘Transfer to PFF-101’ in procedure ‘P-1’ (see Figure 2.21).

Next, click **OK, Next Operation** to move to the ‘Operation Data’ dialog for Cake Wash operation ‘CAKE-WASH-1’.

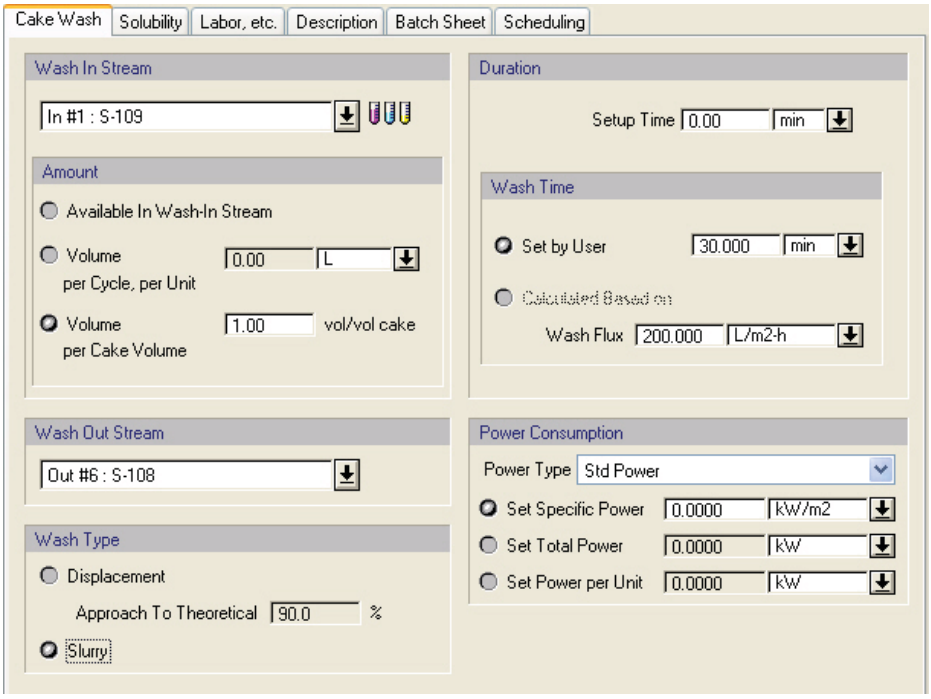


Figure 2.22: The ‘Cake Wash’ tab for Cake Wash operation ‘CAKE-WASH-1’ in procedure ‘P-2’.

In the ‘Cake Wash’ tab (see Figure 2.22), you will need to specify which stream will provide the wash solvent and which one will remove the waste. For this example, keep stream ‘S-109’ as the wash-in stream and select stream ‘S-108’ as the wash-out stream. In addition, you will need to specify what solvent will be used for the wash. To do this, click **View/Edit Stream Composition and/or Amount** ( ) to open the simulation data dialog for the wash-in stream. Add pure component ‘Heptane’ to the stream and click **OK** to return to the operating conditions tab. Notice that you can choose among three specification options for the volume of wash to use:

- Available In Wash-In Stream,
- Volume per Cycle, per Unit, or
- Volume per Cake Volume.

If the first option is selected, the program will use the amount that is available in the wash-in stream as the wash amount. Therefore, you must specify the mass or volume of the wash-in stream through the stream’s simulation data dialog. Alternatively, you can select the second

option and specify the volume of wash to use per procedure cycle and per equipment unit directly, or select the third option and specify the specific volume of wash with respect to the cake volume. For this example, please keep the third option (which is the default one) and change the value of the volume per cake volume to one. Keep the default values for the wash time (30 minutes) and the wash flux (200 L/m^2-h), and change the wash type from 'Displacement' to 'Slurry'. A "slurry" wash will essentially dilute the soluble components trapped in the cake and remove most of them in the wash stream, whereas a "displacement" wash will remove the soluble components from the cake in a plug-flow fashion.

Finally, click **OK, Next Operation** to initialize the Transfer Out operation (named 'TRANSFER-OUT-1') in this unit procedure. In this operation, you will need to specify that you are going to transfer out the cake using a specific stream (the 'Cake' stream is the only choice in this case) and the transfer will be done at a certain rate (10 kg/min in this case). Also, please specify a setup time of 20 minutes for this operation. Then, click **OK** to return to the flowsheet.

You have now finished initializing the operations and streams for this example process. Click **Save** on the **File** menu to save your work.

2.1i Simulating the Process and Viewing the Simulation Results

SOLVING MASS AND ENERGY BALANCES

At this point, you can click **Solve M&E Balances** on the **Tasks** menu to perform the simulation. This will cause the program to perform the mass and energy balances for the entire process, estimate the sizes of all pieces of equipment that are in 'Design Mode', and model the scheduling of each piece of equipment. As a shortcut for performing simulations, you may hit **Ctrl+3** or **F9**, or simply click **Solve ME Balances** () on the **Main** toolbar.

VIEWING SIMULATION RESULTS

The following simulation results can then be viewed for this example:

Stream Data

The calculated flowrates and compositions of intermediate and output streams can be viewed by revisiting the corresponding simulation data dialog windows (double-click on any stream line to see its simulation data dialog).

Procedure Data

The procedure start time, end time, and cycle time (its duration), as well as throughput analysis results for a procedure, can be viewed by visiting the corresponding 'Procedure Data' dialog (right-click on the desired unit procedure icon and click **Procedure Data** on the context menu of that procedure).

Operation Data

The calculated parameters for an operation can be viewed by visiting the corresponding 'Operation Data' dialog (right-click on the desired unit procedure icon and choose the operation you are interested in from the **Operation Data** context menu). For instance, you

can see how long each of the charge operations takes (recall that their durations were based on a given mass to be charged and a flowrate).

Equipment Contents

The contents of a piece of equipment as a function of time can be viewed by right-clicking on a unit procedure and selecting **Equipment Contents** or **Procedure Activity Overview** on the context menu of that procedure.

Streams & Material Balance Report (SR)

A report containing information on raw material requirements, stream compositions and flow rates, as well as an overall material balance, can be generated and displayed by clicking **Streams & Mat. Balance (SR)** on the **Reports** menu. This report includes an overview of the process, a listing of the raw material requirements, a listing of the compositions of each stream, and an overall component balance. Please generate and view this report now. To see more comprehensive stream reports, please refer to the synthetic pharmaceutical example (see 2.2e Process Analysis), the β-Galactosidase example (see 2.3e Process Analysis) and the industrial wastewater treatment example (see 2.4b Process Analysis). If you wish to customize the stream report, click **Options** on the **Reports** menu and switch to the 'Stream' tab; for more details on reports, see Chapter 12 (Reports).

Equipment Data.

To see the calculated number and size of equipment units, right-click on a unit procedure icon and click **Equipment Data** on the context menu of that procedure. This will bring up the 'Equipment' Data dialog of the equipment resource that hosts that procedure. At this point, please open the 'Equipment Data' dialog for Plate & Frame Filter 'PFF-101' (shown in Figure 2.23).

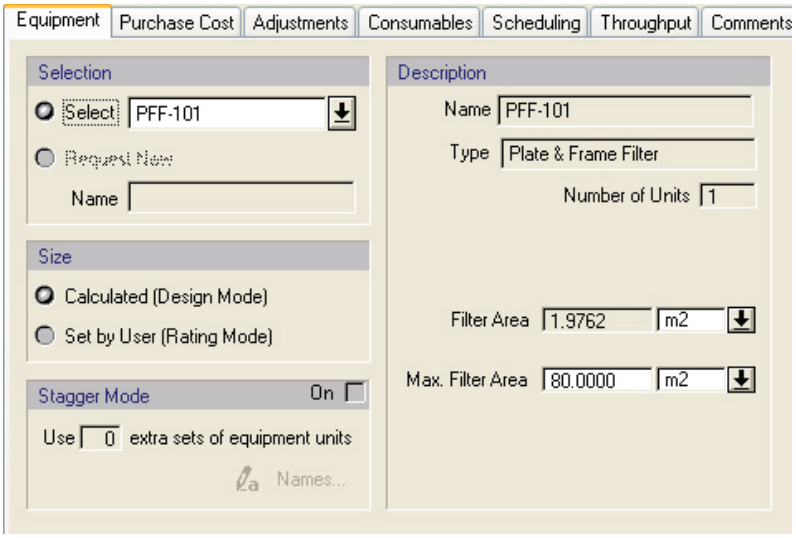


Figure 2.23: The Equipment tab for Plate & Frame Filter 'PFF-1'.

All unit procedures have two options for equipment sizing:

- Calculated (Design Mode), and
- Set by User (Rating Mode).

These options can be specified through the 'Equipment' tab of the corresponding 'Equipment Data' dialog. By default, all equipment resources start in 'Design Mode'. In this mode, SuperPro Designer will determine the required number and size of equipment units based on operating conditions and performance requirements.

Usually, there are physical limitations on the available size of processing equipment. For example, a Plate & Frame Filter may not be available with a cloth area greater than 80 m^2. When you are in 'Design Mode', you must specify the maximum available size for the equipment involved (e.g., the 'Max. Filter Area' for the Plate & Frame Filter). If the calculated equipment size exceeds the maximum allowable size, SuperPro Designer will employ multiple pieces of equipment (sized equally) with sizes that do not violate the maximum available size. For your example process, a filter size of roughly 2 m^2 should have been calculated, as shown in Figure 2.23 (see also file 'GettingStarted8_0a' in subdirectory 'Examples\Misc'). This number was calculated from the volume of material that was processed per cycle, the filtrate flux, and the filtration time.

If you change the equipment sizing method to 'Rating Mode', you can specify the size and number of units. SuperPro Designer will then take this information into account in the simulation calculations (equipment size and number of units may affect the material and energy balances, the process time, etc.). Switching to 'Rating Mode' may also affect the interface of some operations of that procedure. To experience this, please select 'Rating Mode' for Plate & Frame Filter 'PFF-101', change the size of the filter to 4 m^2 and click **OK** to return to the flowsheet. Then, revisit the dialog of the filtration operation. In this case, you need to specify either the filtration time or the average filtration flux (remember that in 'Design Mode' you must specify both). Please set the filtrate flux to 150 L/m^2-h and redo the mass & energy balance calculations. This will calculate a new filtration time (see Figure 2.24). In general, most batch operations have the capability of calculating their cycle time when the equipment size is specified ('Rating Mode').

Through the 'Equipment' tab, you can also select the specific piece of equipment that is going to carry out the processing step. By default, it is assumed that each unit procedure is carried out in its own (exclusive) equipment. However, two or more different unit procedures can share equipment if they are in batch operating mode and the entire process is also in batch mode. For more information on equipment sharing, see 6.1b Equipment Selection & Sharing and the two detailed examples that follow (2.2 The Synthetic Pharmaceutical Process and 2.3 The b-Galactosidase Process).

At this point you have completed the basic initialization steps for the streams, operations, and equipment. As you become more familiar with SuperPro Designer, it will take much less time to do these activities. For instance, all the steps that we have done thus far in this section could

be performed in about 15 minutes if you were already familiar with how to use SuperPro Designer.

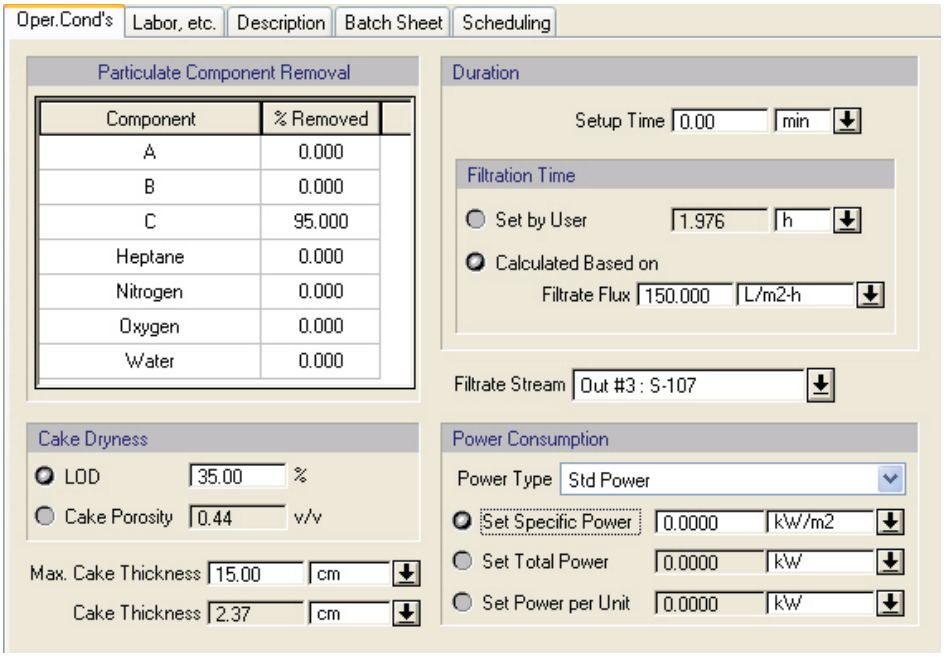


Figure 2.24: The 'Oper. Cond's' tab for Cloth Filtration operation 'FILTER-1' in procedure 'P-2' when the equipment is in 'Rating Mode'.

Important note about building and initializing large process flowsheets *– when you attempt to simulate complex processes, keep in mind that you don't have to add all the unit procedures at once. You can always add or remove procedures as desired at a later stage. For complex processes, it is highly recommended that you begin your simulation with just a handful (core) unit procedures and add more only after you have successfully completed the simulation for the first phase (streams and operations have been initialized correctly and your mass balances make sense).*

USING BREAKPOINTS

When simulating large processes it is sometimes useful to solve only part of the process. Setting breakpoints tells the simulator to halt calculations at a certain point. A brief description of this facility is given below.

You can place a breakpoint, and force the M&E balance execution sequence to pause either right before, or right after the solution of a unit procedure. You may even place a breakpoint inside the unit procedure's solution sequence of unit operations.

▶ To Place a Breakpoint on a Unit Procedure...

1. Right click on a unit procedure to bring up its context menu and select **Set Breakpoints**. Through the 'Breakpoints' dialog that appears, you can specify where to break the simulation of the selected unit procedure.

2. Check the place(s) where you wish the simulation to pause and exit this dialog. Notice that red signs ( ) are shown above the procedure's icon to indicate that one or more breakpoints are set on this procedure. The position of the sign indicates whether the break is on the entry (left sign), operations (middle sign) or exit (right sign) of the procedure.

Once a breakpoint is set, next time the 'Solve M&E Balances' command is issued, the simulation calculation sequence will pause at that location. When the simulation sequence is paused, some buttons of the 'Solve' toolbar become active. Also notice that while the simulation has been paused, all unit procedure display another icon underneath that indicates the simulation state of each procedure at that time (as the simulation is paused). The following sequence of images indicate the state of the unit procedure that is *currently being solved*:

Image	Explanation
	A break on entry has been encountered.
	A break on operation has been encountered.
	A break on exit has been encountered.
	A break on entry has been encountered (shown when there are operations that can auto-adjust the flow of process input streams).
	A break on material pull-in has been encountered (for operations that can auto-adjust the flow of process input streams).
	A break on operation has been encountered (shown when there are operations that can auto-adjust the flow of process input streams).
	A break on material pull-out has been encountered (for operations that can auto-adjust the flow of process output streams).
	A break on exit has been encountered (shown when there are operations that can auto-adjust the flow of process input streams).

The following sequence of images indicate the state of *all other unit procedures* while the simulation is paused:

Image	Explanation
	The procedure has not been visited yet.
	The procedure has been successfully simulated already.
	The procedure's M&E balances are being solved recursively (as part of loop convergence).
	The solution of the procedure's M&E balances ended unsuccessfully (as part of an un-converged loop).
	The solution of the procedure's M&E balances ended unsuccessfully (an error was encountered)

Notes

1. You can toggle the visibility of the breakpoint icons (above the unit procedure) and of the state icons (below the unit procedure) using the **Show / Hide Breakpoints** ( ) and **Show / Hide Status** ( ) buttons, respectively, on **the Simulation Control** toolbar.
2. To temporarily deactivate breakpoints (without removing them), simply visit the 'Breakpoints' dialog of a unit procedure and click once more on the checked breakpoint location. Notice how the checkmark now is still there, but looks faded (grayed out). The breakpoint sign above the unit procedure icon will look faded as well.
3. When the 'Solve M&E Balances' sequence is paused, you may visit the simulation data dialog of any stream, unit procedure, equipment, or operation, to inspect or even modify values of operating conditions. If you modify the values of streams and/or operations belonging to unit procedures that have already been solved (i.e., the check mark icon appears underneath) or to the unit procedure that is currently being solved but the operation whose values have been modified has already been solved, then the new values will not be taken into account until the next 'Solve M&E Balances' command is issued.

CONVERGENCE OF RECYCLE LOOPS

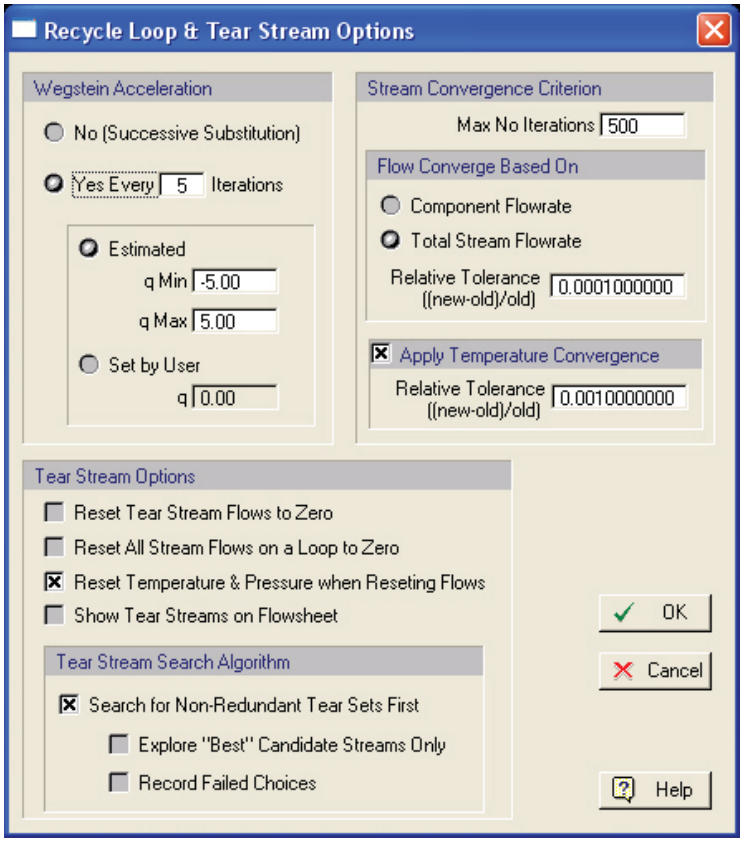


Figure 2.25: Adjusting the convergence parameters in a process that includes recycle loops.

The material of this paragraph is only relevant to process flowsheets that include recycle loops. To see an example of a recycle loop, please open file Bgal8_0b that can be found in the Examples \ Bgal directory of SuperPro Designer. In this file, streams 'S-102' and 'S-108' are part of a recycle loop. For a description of this file, see2.3 The b-Galactosidase Process.

SuperPro Designer's default convergence parameters for flowsheets that include loops (which result in iterative calculations) have been tuned in order to be adequate for most situations. However, occasionally (especially in cases involving highly non-linear models) they may fail to converge. In these cases, you may fine-tune the convergence characteristics for a particular application. To change the convergence parameters for the process with loops, click **Process Options ▸ Recycle Loop & Tear Stream Options** on the **Edit** menu. Alternatively, right-click on the flowsheet and click **Recycle Loop & Tear Stream Options** on the flowsheet's context menu.This will bring up the 'Recycle Loop and Tear Stream Options' dialog of Figure 2.25.

Below is a list of actions that you can take to improve the system's performance in converging iterative calculations:

1. Adjust the convergence tolerance ('Relative Tolerance') for stream total or component mass flow and, optionally, temperature. The convergence tolerance is defined as (new value - old value) / old value. Setting the relative tolerance to a larger value may speed up the convergence (but may lead to less accurate simulation results).
2. Switch from convergence based on the total flow to convergence based on individual component flows. This may slow down the convergence process but it will yield more accurate simulation results. This is especially important for process files that deal with components that are in trace amounts, but whose accurate balance is of utmost importance (e.g., hazardous and/or toxic chemicals).
3. Increase the maximum number of iterations.
4. Request that tear streams be initialized to zero flow (for all components) before every new simulation. Normally, in cases where the process simulation has been converged once, the initially guessed state for tear streams is their current state at the end of the previous (converged) simulation. In most cases, this leads to a faster convergence the next time the mass and energy balances are solved. However, after a convergence failure, it may be better to start with zero values.
5. Adjust the Wegstein algorithm parameters (q_{min}, q_{max}, and q). If the convergence procedure seems to be unstable, raising the value of q_{min} (i.e., making it less negative) may improve convergence; if it is converging very slowly but monotonically, you might lower q_{min}; and if it is converging in an oscillatory manner, try raising q_{max}. You also have the option of adjusting the value of q. If q is between zero and 1, the procedure is a modified successive substitution; if q is negative then the convergence is accelerated.
6. Switch from Wegstein acceleration to successive substitution. This may slow down the convergence calculations but will increase the likelihood of convergence.
7. Select a different tear stream for a recycle loop by right clicking on a specific stream (that is part of the loop) and selecting 'Preferred Tear'. The current tear streams are identified on the flowsheet (with two red slashes) if you check the 'Show Tear Streams on Flowsheet' option that is available in the 'Recycle Loop and Tear Stream Options' dialog.

2.1j Setting the Process Scheduling Information

The following terms are used for batch process scheduling:

Term	Description
Annual Operating Time (AOT)	The number of hours per year the plant is devoted to making a specific product.
Campaign	An uninterrupted run of batches.
Batch Time	The start to finish time for a single batch.
Cycle Time	The time between two consecutive batch starts. It is sometimes called the recipe or plant cycle time.
Minimum Cycle Time	The minimum possible cycle time based on the time (scheduling) bottleneck.
Cycle Time Slack	The difference between the actual and minimum cycle times.

If the process is in batch mode (as is the case for your example process), you should provide process scheduling information before performing a simulation. SuperPro Designer allows you to specify the following scheduling data:

1. For each operation:
   (a) the process time,
   (b) the setup and turnaround times, and
   (c) the starting time.
2. For each procedure, the number of cycles.
3. For the entire plant:
   (a) the available AOT,
   (b) the number of campaigns per year,
   (c) the number of batches per year, and either:
   (d) the cycle time, or
   (e) the cycle time slack.

Scheduling of operations was explained in Section 2.1h Initializing Unit Procedures. In that section, the 'Scheduling' tab of a filtration operation was shown in Figure 2.21. Through the 'Scheduling' tab, you can specify the start time of an operation relative to the beginning of a batch or relative to the start or end of other operations in the same procedure or in a different procedure. You may also specify the process time (if it is not calculated by the model), the setup time and the turnaround time for an operation.

To specify the number of cycles per batch for a procedure (the same number applies to all operations of the procedure), simply right-click on the unit procedure's icon and select **Procedure Data** from the corresponding context menu. By default, all procedures start with one cycle.

To specify scheduling information for an entire process, click **Recipe Scheduling Information** on the **Tasks** menu. This will bring up the 'Recipe Scheduling Information' dialog (see Figure 2.26 below).

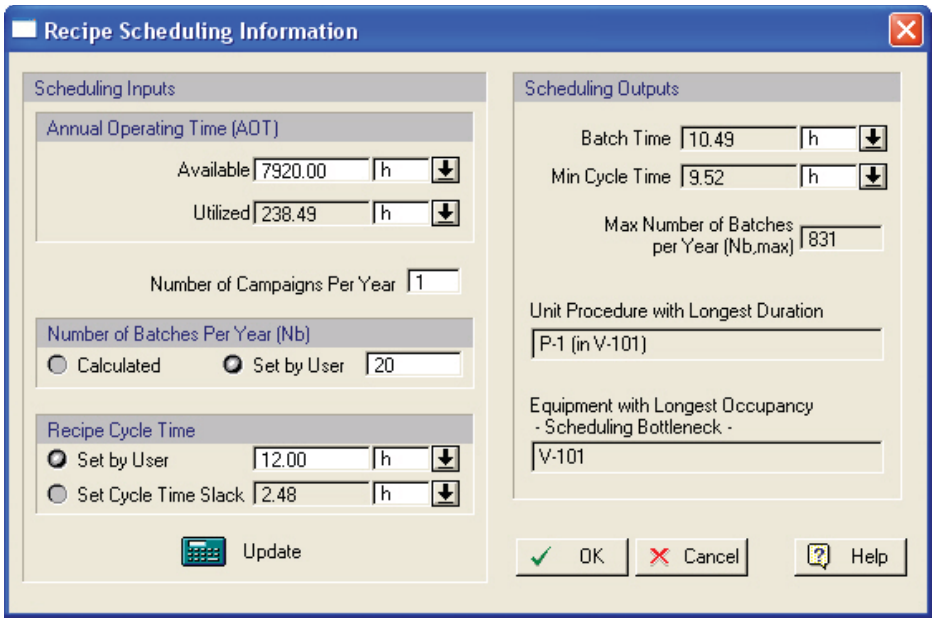


Figure 2.26: Specifying the scheduling information for a batch process.

For your example process (simulated in 'Design Mode'), please change the number of batches per year to 20. This implies that your example process will be run in a pilot plant 20 times this year (it is assumed that the equipment used by this process is used by other processes the rest of the year). In addition, please change the recipe cycle time for this process to 12 hours to reflect the completion of one batch during every 12-hour shift and of the whole process in approximately 240 hours. Click **Update** ( ) to see the actual annual operating time (AOT) that the plant is utilized by this process.

Based on the scheduling information and the available AOT specified for the plant, the system will do the following:

1. Make sure there is no conflict created by the specified start time and end time of processing steps. Conflicts can be created if the cycle times of procedures that share equipment overlap.
2. Make sure there is no conflict between the specified available AOT, the specified or calculated number of batches, and the specified or calculated recipe cycle time.
3. Calculate the number of batches (if not set by user), the recipe batch time, the recipe cycle time (if not set by user), the recipe cycle time slack (if not set by user), the utilized AOT, the plant's minimum cycle time (with maximum batch overlapping), the maximum number of batches possible, the longest procedure (i.e., the procedure with the longest total cycle time) and the scheduling bottlenecking equipment (the equipment with the longest occupancy time).

2.1k Viewing Scheduling, Equipment Utilization and Resource Tracking Results

A variety of scheduling, equipment utilization and resource tracking tools are included in SuperPro Designer. These include:

- Operations / Equipment Gantt Charts,
- Main and Auxiliary (CIP Skids, SIP Panels) Equipment Occupancy Charts,
- Resource Demand Charts, and
- Resource Inventory Charts.

OPERATIONS / EQUIPMENT GANTT CHARTS

The Operations Gantt Chart and the Equipment Gantt Chart display scheduling and equipment utilization information, respectively, for a batch process recipe in the form of a Gantt Chart. These charts can be generated either for a single batch or for multiple batches using dedicated items on the **Tasks ▸ Gantt Charts** menu. Note that this menu is only available if the plant operation mode is batch (see 2.1c Specifying the Mode of Operation for the Entire Plant).

Please generate the Operations Gantt Chart for your example process and for a single batch by selecting **Gantt Charts ▸ Operations GC** on the **Tasks** menu. It should look similar to Figure 2.27 below. The left view (spreadsheet view) displays the name, duration, start time and end time for each activity participating in the overall scheduling and execution of the recipe. This can be either an elementary activity or an activity summary. In the Operations Gantt Chart, an elementary activity corresponds to an operation executed during a single procedure cycle. For this example, activity summaries are shown for unit procedures and for the complete recipe. You can expand or collapse activity summaries by clicking on the + or – signs in the boxes to the left of activity names. The right view (chart view) displays a bar for each activity, whose horizontal position and length indicate the start time and duration, respectively, of that activity.

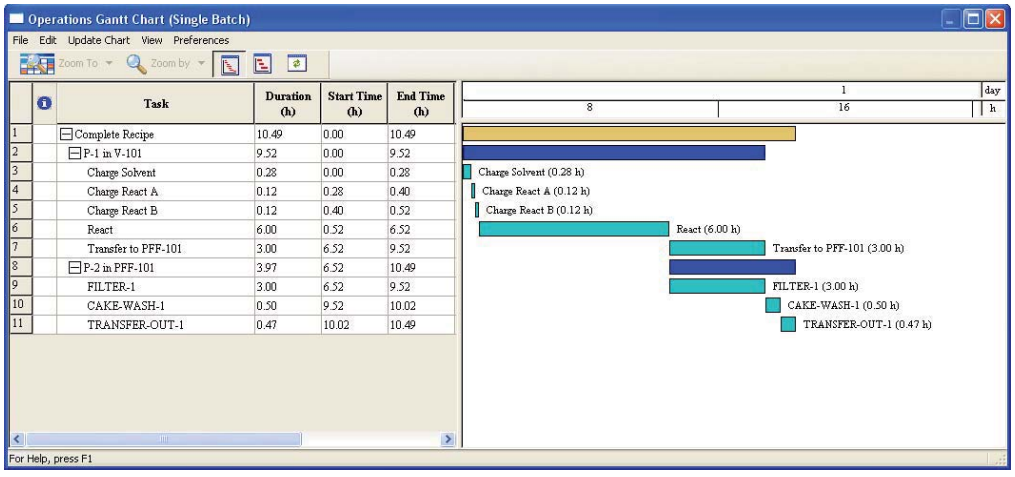

Operations Gantt Chart (Single Batch)
File Edit Update Chart View Preferences
Zoom To
Zoom by
Task
Duration (h)
Start Time (h)
End Time (h)
1 Complete Recipe 10.49 0.00 10.49
2 P-1 in V-101 9.52 0.00 9.52
3 Charge Solvent 0.28 0.00 0.28
4 Charge React A 0.12 0.28 0.40
5 Charge React B 0.12 0.40 0.52
6 React 6.00 0.52 6.52
7 Transfer to PFF-101 3.00 6.52 9.52
8 P-2 in PFF-101 3.97 6.52 10.49
9 FILTER-1 3.00 6.52 9.52
10 CAKE-WASH-1 0.50 9.52 10.02
11 TRANSFER-OUT-1 0.47 10.02 10.49
1 day
8 16 h
Charge Solvent (0.28 h)
Charge React A (0.12 h)
Charge React B (0.12 h)
React (6.00 h)
Transfer to PFF-101 (3.00 h)
FILTER-1 (3.00 h)
CAKE-WASH-1 (0.50 h)
TRANSFER-OUT-1 (0.47 h)
For Help, press F1

Figure 2.27: The Operations Gantt Chart. for a single batch.

The Equipment Gantt Chart interface is similar to that of the Operations Gantt Chart. Please generate the Equipment Gantt Chart for your example process and for a single batch now by clicking **Gantt Charts ▸ Equipment GC** on the **Tasks** menu. In this chart, the elementary

activity corresponds to the time frame that an equipment is kept busy by an operation during a procedure cycle. In this example, activity summaries are shown for unit procedures (corresponding to the time frame that an equipment is kept busy by a procedure), for equipment (corresponding to the time frame that an equipment is kept busy by all procedures it hosts), and for the complete recipe (named 'total occupation time').

In addition to displaying scheduling information, Gantt Chart interfaces also present you with a graphical way to modify scheduling parameters for an activity and immediately visualize the effects on the entire batch production. In fact, anything you can accomplish with the simulation data dialog interfaces described in 2.1h Initializing Unit Procedures and 2.1j Setting the Process Scheduling Information, you can also accomplish from the Gantt Chart interfaces. To do that, simply double-click on a bar, or right-click on a bar and select the uppermost entry on the context menu for that bar. This will display the simulation data dialog for the corresponding activity. For example:

- if the bar corresponds to an operation, it will display the 'Operation Data' dialog for that operation;
- if the bar corresponds to a unit procedure, it will display the 'Procedure Data' dialog for that unit procedure;
- if the bar corresponds to an equipment resource (available only in Equipment Gantt Charts), it will display the 'Equipment Data' dialog for that piece of equipment;
- if the bar is the one at the top of the chart (named 'complete recipe' in Operation Gantt Charts and 'total equipment occupancy' in Equipment Gantt Charts), it will display the 'Recipe Scheduling Information' dialog (see Figure 2.26).

If you change the simulation parameters in the above dialogs, you must click **Redo Calc. & Update Chart** ( ) on the toolbar or **Update Chart** on the chart's main menu. This will solve the mass and energy balances again and have the Gantt chart updated to reflect the new scheduling settings for the recipe.

You can change the style (e.g. bar width, time scale, etc.) and contents (e.g., displayed activity summaries) of a Gantt Chart by selecting **Styles ▸ Gantt Chart** on the **Preferences** menu of the chart. You may also use the items in the **File** menu of the chart to print the chart, export scheduling data to MS-Excel or MS-Project, or export the chart as a Windows Metafile (.wmf). Note also that if you generate an Operations Gantt Chart or an Equipment Gantt Chart for multiple batches, you can change the default number of batches shown on the chart by right-clicking on the chart and selecting **Set Number of Batches** from the chart's context menu.

Please refer to the synthetic pharmaceutical example (see Figure 2.49) and the β-Galactosidase example (see Figure 2.62) to see Gantt Charts for more complex processes. For more information on these charts, see 7.4 The Operations Gantt Chart (OGC) and 7.5 The Equipment Gantt Chart (EGC).

EQUIPMENT OCCUPANCY CHARTS

Another way of visualizing the execution of a batch process as a function of time is through the Equipment Occupancy Chart. This chart shows in a graphical way how long each equipment is kept busy by some operation and how long it is just idle during batch processing. Each chart

can be generated either for a single batch or, preferably, for multiple batches using dedicated items on the **Charts ▸ Equipment Occupancy** menu.

Please generate this chart for your example process by selecting **Equipment Occupancy ▸ Multiple Batches** on the **Charts** menu. By default, two batches are shown. To add more, right-click on the chart to bring up the chart's context menu and select **Set Number of Batches**. Please change the number of batches to three and press **OK**. Your chart should look similar to that shown in Figure 2.28.

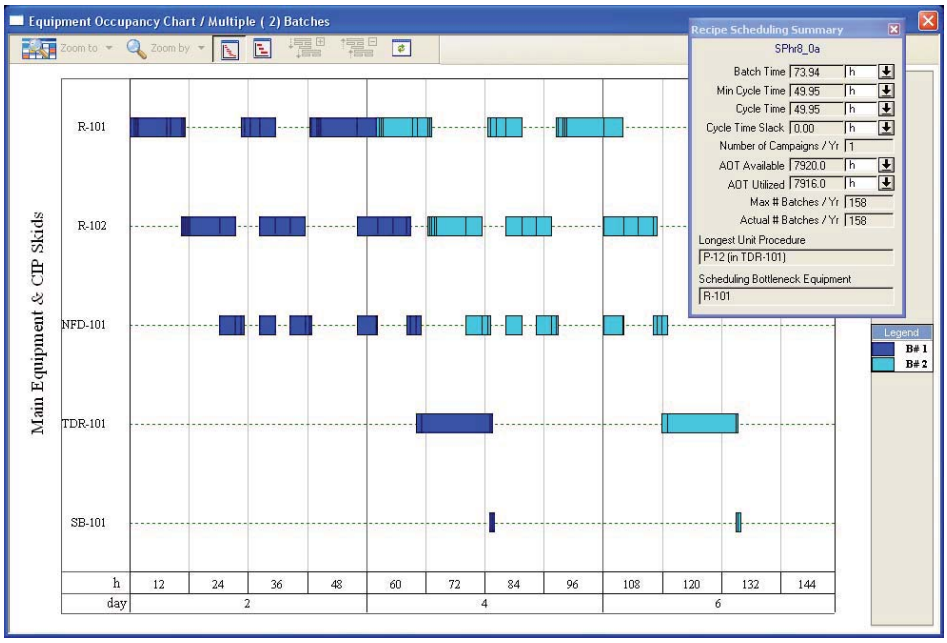


Figure 2.28: The Equipment Occupancy Chart for three consecutive batches.

For each equipment, the occupancy time by some operation is represented by a bar. White space represents idle time. Placing the mouse pointer over a bar will display the name of the operation that corresponds to that bar. Right-clicking on a bar will bring up its context menu. On this menu, you can click **Operation Data** to display the 'Operation Data' dialog for the corresponding operation, or **Procedure Data** to display the 'Procedure Data' dialog for the corresponding unit procedure, or **Equipment Data** to display the 'Equipment Data' dialog for the corresponding equipment. In the 'Scheduling' tab of that dialog, you can see, among others, the total equipment occupancy time per batch.

The equipment with the least idle time between consecutive batches (or, equivalently, the longest occupancy time per batch) is considered the *time (or scheduling) bottleneck* (V-101 in this case). This is the equipment that determines the maximum number of batches per year. Its occupancy time per batch (9.52 hours in this case) corresponds to the minimum cycle time of the recipe (the minimum possible time between two consecutive batch starts). The total equipment occupancy time per batch (12 hours in this case) corresponds to the actual cycle time of the recipe (the actual time between two consecutive batch starts). To view this information, right-click on an empty area in the chart to bring up the chart's context menu and check **Scheduling Summary**. This will display the 'Recipe Scheduling Summary' dialog for

the process. That dialog presents (for display purposes only) the same information as the 'Recipe Scheduling Information' dialog of Figure 2.26. To change the style and contents of the Equipment Occupancy Chart, right-click on an empty area in the chart to bring up the chart's context menu and select **Edit Style**.

Please refer to the synthetic pharmaceutical example (see Figure 2.50) and the β-Galactosidase example (see Figure 2.58) to see Equipment Occupancy Charts for more complex processes. For more information on Equipment Occupancy Charts, see 7.6 The Equipment Occupancy Chart (EOC).

RESOURCE DEMAND CHARTS

In addition to creating Gantt charts for equipment utilization and operations, SuperPro Designer automatically generates graphs of resource demand as a function of time for such things as raw materials, labor, heating and cooling utilities, and power. These can be accessed through the **Charts** menu. For instance, to view the labor demand for this example process, select **Labor ▸ Multiple Batches** on the **Charts** menu. Next, in the labor resource selection dialog that pops-up, keep the default selection ('Operator') and click **OK**. Figure 2.29 displays the 'Operator' labor resource demand graph for two consecutive batches. To add more, right-click on the chart to bring up the chart's context menu and select **Set Number of Batches**. As shown in this chart, two operators are required to handle this process. If you move the cursor close to a peak, SuperPro Designer displays the operations that create that peak.

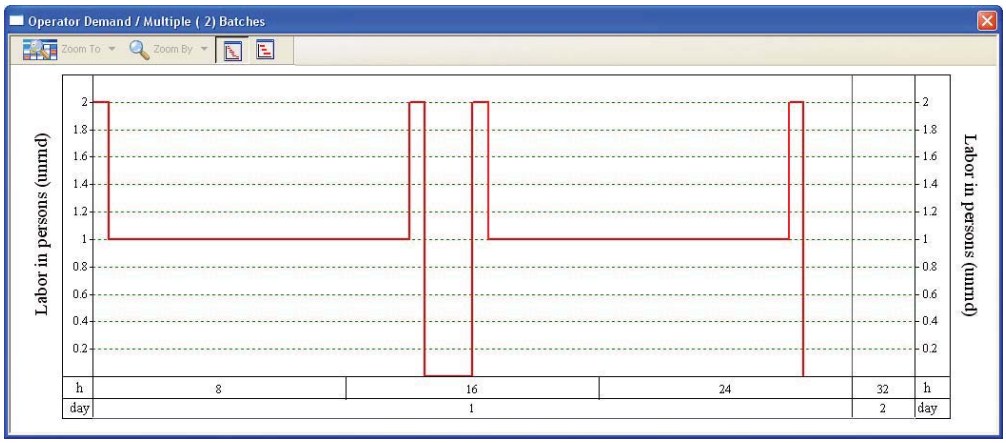


Figure 2.29: The 'Operator' labor resource demand chart for the example process.

To change the contents (variables displayed) and style (e.g., color, thickness, etc.) of a resource demand graph, right-click on the chart to bring up its context menu and select **Edit Style**. Through context menu commands you can also print a chart, export a chart as a Windows Metafile (.wmf), or export its data into a file in Excel format with a discretization time interval that can be specified by the user. This is a useful feature if you wish to combine demands for a certain resource from multiple process files in Excel.

Please refer to the synthetic pharmaceutical example (see Figure 2.51) and the β-Galactosidase example (see Figure 2.63) to see resource demand charts for more complex processes.

RESOURCE INVENTORY CHARTS

SuperPro Designer can also analyze and display inventory information for material resources. Recall that 50 kg of material 'A' are used in each batch. Suppose that there is a 300kg storage capacity for 'A' and an opening inventory of 100kg. Suppose further that the loading rate of material 'A' into storage is 200 kg/h. How often should shipments of 'A' be scheduled? Please select **Materials ▸ Entering, Inventory ▸ Multiple Batches** on the **Charts** menu. Select pure component 'A' from the pure components drop-down list box and click the **Supply Info** button. This will bring up the 'Resource Inventory Data' dialog for the selected ingredient. Fill out the dialog as shown in Figure 2.30. This will tell SuperPro Designer that the supply of material 'A' should be replenished when the inventory falls to 10% (or 30 kg) of the capacity. The replenishment should be halted when the inventory reaches 85% (or 255 kg) of storage capacity. Click **OK** to return to the previous dialog.

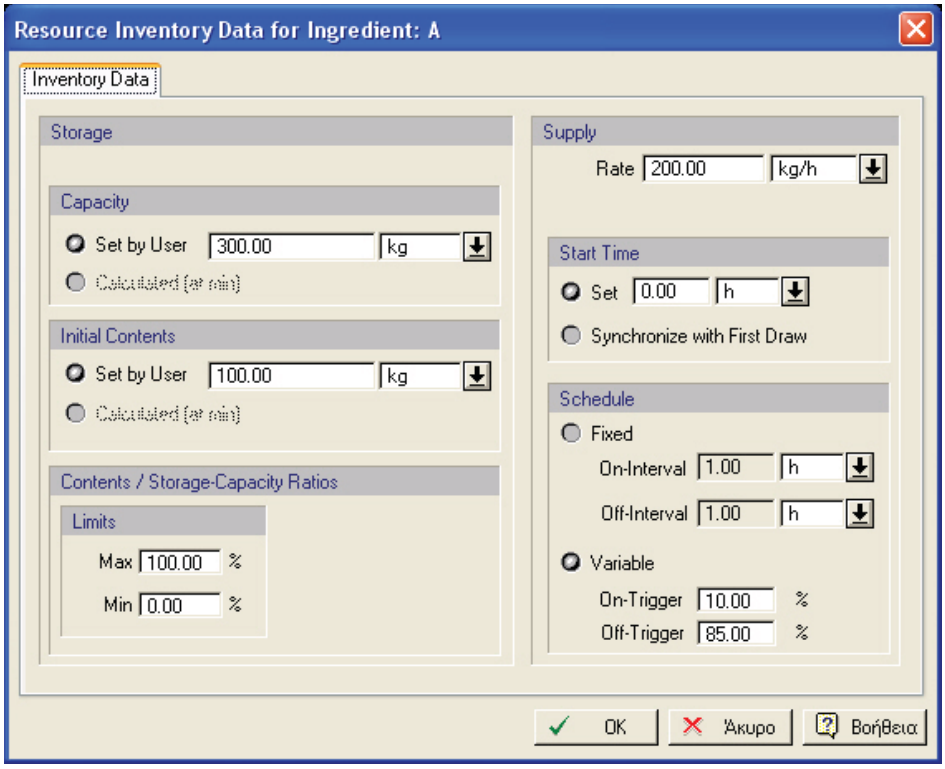


Figure 2.30: The Resource Inventory Data dialog.

Next, click the **Chart Style** button to bring up the 'Inventory Chart Style' dialog. Switch to the 'Time Line' tab and click the **Edit** button. In the 'Default Time Line Style' dialog that comes up, change the minor time units count to 12 hours (the recipe cycle time) and click **OK** to return to the previous dialog. This will make observation of batches easier since a new batch cycle starts every 12 hours in this example. Click **OK** again to continue and the chart will be displayed with two batches. Set the number of batches to 12 by right-clicking on the chart and selecting **Set Number of Batches** from the context menu that pops up. The resulting chart will look like that of Figure 2.31. The brown line corresponds to the inventory level and the

aqua line corresponds to the supply rate of material ‘A’. The increases in inventory indicate the replenishment schedule suggested by SuperPro Designer.

To explain this further, let us focus first on the first batch cycle. Please click the **Show Chart at Nominal Size** button and then the **Zoom To** button on the chart’s toolbar and check the **Day** option. The chart will zoom to one day. Notice that the supply of fresh material starts right away since the opening inventory (100 kg) is less than 85% of storage capacity (255 kg). The inventory amount increases linearly up to the point that a charge of material starts as part of operation ‘Charge React A’. During charge, 50 kg of material are being charged and at the same time fresh material is being supplied at a lower rate, which results in a linear decrease in inventory amount. Afterwards, the inventory amount increases linearly again until it reaches the 85% limit, which triggers material supply off. The inventory amount remains at the same level until new material is charged. In subsequent batch cycles, every time material is charged, the inventory amount falls by 50 kg. This leaves 55 kg in the beginning of the sixth batch cycle. During charge in that cycle, the inventory amount reaches 10% of storage capacity (30 kg), which triggers the supply of fresh material on, while the charge of material is on-going. This results in a linear decrease in the inventory amount during charge in the sixth batch cycle (please scroll down to the 3rd day to observe this). Afterwards, the inventory amount increases linearly again until it reaches 85% of storage capacity and material supply is triggered off again. The above replenishment schedule is repeated every sixth batch cycle.

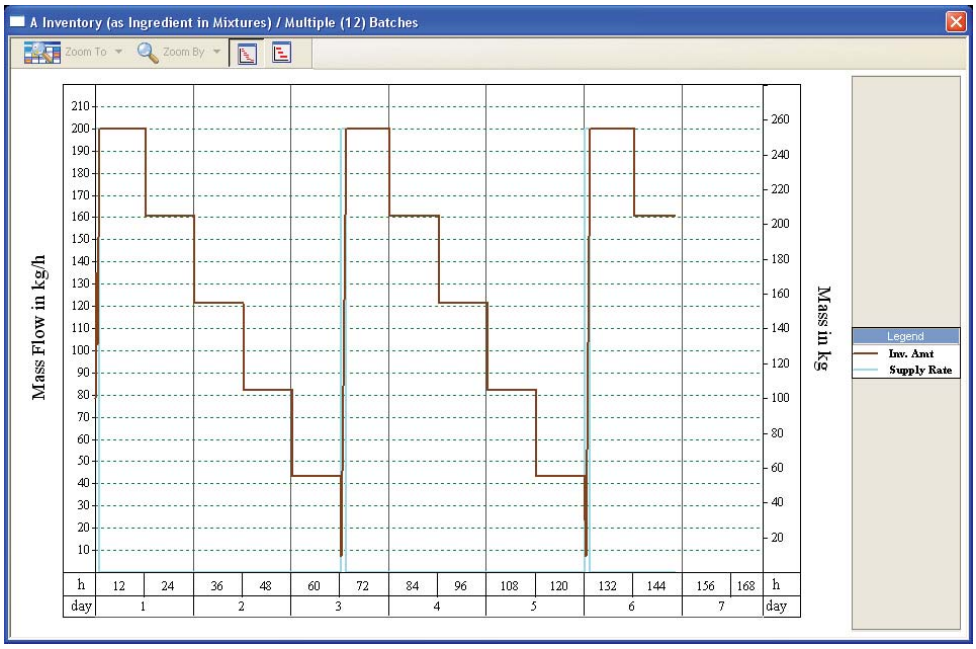


Figure 2.31: The inventory profile of pure component ‘A’ in the example.

Note that you can see the exact time and value of a point in a line by placing the mouse pointer over that point. By default, the inventory graph displays the inventory amount and the supply rate. To change the contents (variables displayed) and style (e.g., color, thickness, etc.) of the graph, right-click on the chart to bring up its context menu and click **Edit Style**. Through other context menu commands, you can print a chart, export a chart as a Windows Metafile (.wmf),

or export chart data into a file in Excel format with a discretization time interval that can be specified by the user. This is a useful feature if you wish to combine demands for a certain resource from multiple flowsheets in Excel.

2.1l Throughput Analysis and Debottlenecking

SuperPro Designer is equipped with powerful throughput analysis and debottlenecking capabilities. The objective of these features is to allow the user to quickly and easily analyze the capacity and time utilization of each piece of equipment, and to identify opportunities for increasing throughput with the minimum possible capital investment. The most important features are:

- the Utilization Factors chart, and
- the Batch Size Potential chart, which indicates opportunities for increased production per batch.

For a detailed throughput analysis example (based on the process of the second example), see Chapter 11 (Debottlenecking). A brief description is given here.

Since throughput calculations are based on fixed equipment, set all pieces of equipment to 'Rating Mode'. Specify 1630 L for the reactor and 2 m^2 for the filter (as was done for file 'GettingStarted8_0b' in subdirectory 'Examples\Misc'). Then, solve the model.

UTILIZATION FACTORS CHART

Select **Throughput Analysis ▸ Utilization Factors** on the **Charts** menu. The Utilization Factors chart shown below will appear.

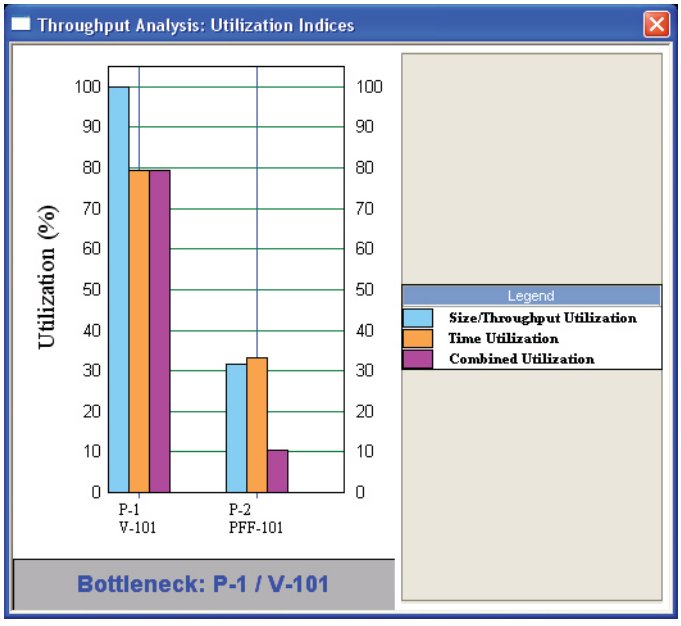


Figure 2.32: The Utilization Factors Chart.

The chart shows, for each unit procedure, the capacity (size) utilization (how "full" the equipment is) and the time utilization (its "uptime" or "busy time") of the hosting equipment.

This information is also available in the ‘Throughput’ tab of the ‘Procedure Data’ dialog for each unit procedure. Note that the time utilization is somewhat low because some slack time was introduced (see Figure 2.26). The combined utilization is the product of the two. A batch size (throughput) bottleneck corresponding to the limiting procedure/equipment combination in terms of highest combined utilization (‘P-1/V-101’ in this case) is also indicated on the chart.

BATCH SIZE POTENTIAL CHART

Furthermore, estimates of batch size (throughput) potential are available in the Batch Size Potential chart. To create this chart, you must first select a throughput reference rate for batch size calculations. To do that, select **Rate Reference Flow(s)** on the **Tasks** menu to open the ‘Rate Reference Flows’ dialog and switch to the ‘Throughput’ tab. Please choose the total flow of the ‘Cake’ stream as reference, and specify the word “Cake” as the quick reference symbol. Then click **OK** to close this dialog.

Subsequently, select **Throughput Analysis ▸ Batch Size Potential** on the **Charts** menu to view the batch size potential chart using the total flow of the ‘Cake’ stream as throughput reference rate (see Figure 2.33). This chart shows the actual batch size (red dotted lines) and three estimates (conservative, realistic, and theoretical) of batch size potential for each procedure/equipment combination. A size bottleneck based on each estimation method is also indicated on the chart. This corresponds to the procedure/equipment combination that has the smallest batch size potential based on that method. In this example, ‘P-1/V-101’ is the size bottleneck based on any estimation method. For each unit procedure, the above information can also be found in the ‘Throughput’ tab of the corresponding simulation data dialog.

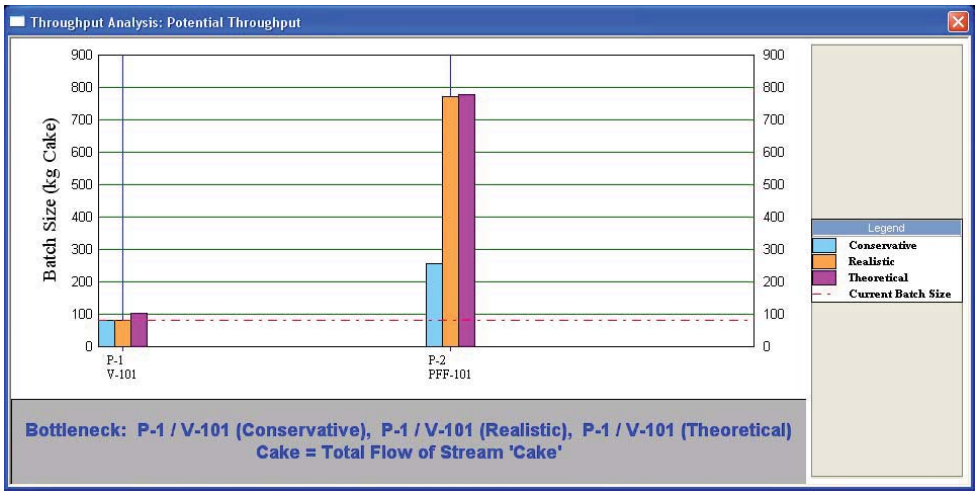


Figure 2.33: The Batch Size (Throughput) Potential Chart.

To omit an equipment resource from the throughput analysis and, thereby, from the above charts, open the corresponding ‘Equipment Data’ dialog, switch to the ‘Throughput’ tab, and check the option named ‘Omit from Throughput Analysis’. For display purposes, a relevant specification setting will be checked in the ‘Throughput’ tab of all unit procedures that utilize that equipment resource.

2.1m Cost Analysis and Economic Evaluation

SuperPro Designer performs thorough cost analysis and economic evaluation calculations and generates three pertinent reports. The key initialization steps are described below using our simple process as an example (see also file 'GettingStarted8_0b' in the 'Examples\Misc' subdirectory of SuperPro Designer).

For a detailed description of cost analysis and economic evaluation, please consult Chapter 9 (Economics).

SUPPLYING REVENUE, RAW MATERIAL, AND WASTE STREAM DATA

This step must precede economic evaluation and environmental impact assessment calculations. Please select **Stream Classification** on the **Task** menu. You will be presented with a dialog window (see Figure 2.34) where you can classify all input and output streams as raw materials, revenues or wastes (solid, aqueous, organic, or gaseous) and supply any cost data associated with the classification. By default, the system estimates a purchase or selling price for a stream based on the price of each component and the composition of the stream. The price of a pure component or stock mixture is part of its properties, which can be edited when registering components as described in 2.1e Registering Components and Mixtures.

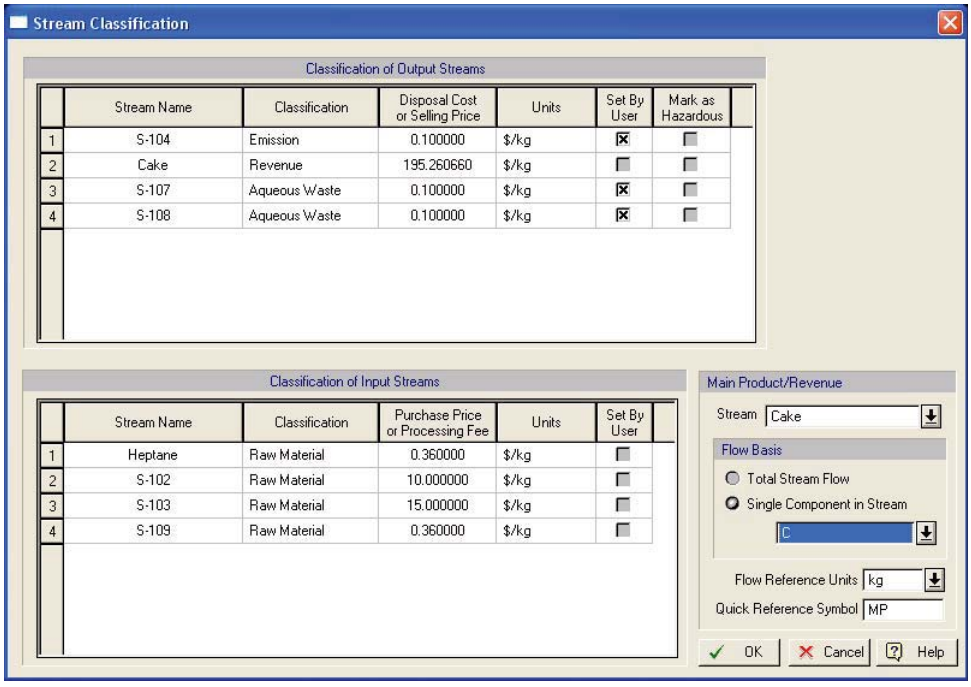

Stream Classification
Classification of Output Streams
Stream Name | Classification | Disposal Cost or Selling Price | Units | Set By User | Mark as Hazardous
1 S-104 Emission 0.100000 $/kg
2 Cake Revenue 195.260660 $/kg
3 S-107 Aqueous Waste 0.100000 $/kg
4 S-108 Aqueous Waste 0.100000 $/kg
Classification of Input Streams
Stream Name | Classification | Purchase Price or Processing Fee | Units | Set By User
1 Heptane Raw Material 0.360000 $/kg
2 S-102 Raw Material 10.000000 $/kg
3 S-103 Raw Material 15.000000 $/kg
4 S-109 Raw Material 0.360000 $/kg
Main Product/Revenue
Stream Cake
Flow Basis
Total Stream Flow
Single Component in Stream
C
Flow Reference Units kg
Quick Reference Symbol MP
OK
Cancel
Help

Figure 2.34: The 'Stream Classification' dialog.

In this example process, please classify the output streams and set costs for the two liquid waste streams as shown in Figure 2.34. First, specify that the 'Cake' stream is a revenue stream. Notice that the 'Selling Price' of a revenue stream is calculated automatically, based on the stream's composition (recall that there is still heptane and small amounts of impurities in our product cake, so the price per kg of cake is less than the $300/kg price of pure component 'C'.)

Next, classify the two liquid waste streams as aqueous waste. Check the ‘Set By User’ options next to the emission stream and the two liquid waste streams and type in a value of $0.10/kg for the ‘Disposal Cost’ of each. Finally, select the ‘Cake’ stream as the ‘Main Product/Revenue’ stream from the corresponding drop-down list, and specify that the unit cost for this process will be reported based on the component flow of product ‘C’.

Note that the classification of a stream as a solid waste, aqueous waste, organic waste, or an emission will cause it to be reported in dedicated sections of the Environmental Impact Report, where a detailed bookkeeping is kept on all chemicals that end up in each waste category. Specifically, streams that are connected to venting ports are already classified as emission streams by default. The Environmental Impact Report allows you to evaluate the burden of the process on the environment. Such an assessment assists the designer to focus his/her attention on the most troublesome streams and the processing steps that generate them. A related report, the Emissions Report (EMS) provides information on emissions of volatile organic compounds (VOC) and other regulated compounds. The Emissions Report will also give information on the emitted components as well as the contributing unit procedures and operations to these emissions.

ADJUSTING THE COST FACTORS

The user can specify economic evaluation parameters at four levels:

- the Operation level,
- the Equipment level,
- the process Section level, and
- the Process level.

Please note that the economic evaluation parameters from each of the three levels have a significant impact on the cost calculations. Therefore, the parameters at all three levels should be examined by the user and edited if necessary.

ECONOMIC PARAMETERS AT THE OPERATION LEVEL

Parameters that affect demand for labor and utilities are specified at the operation level. For instance, the labor requirement for an operation can be specified through the ‘Labor, etc.’ tab of an operation’s data dialog. Through the same dialog you can specify auxiliary utilities, which have no impact on material and energy balance calculations (they do not affect output stream temperatures). They are only considered in costing and economic evaluation calculations. Auxiliary utilities offer a convenient way to associate utility consumption with generic boxes and other operations that do not calculate utility demand.

ECONOMIC PARAMETERS AT THE EQUIPMENT LEVEL

All equipment resources have two common dialog tabs through which the user can provide information that affects the capital investment and certain operating cost items. Information about equipment purchase costs and various adjustments can be provided through the ‘Purchase Cost’ and ‘Adjustments’ tabs of the ‘Equipment Data’ dialog.

Equipment Purchase Cost

Figure 2.35 shows the 'Purchase Cost' tab for Stirred Reactor (CSTR) 'V-101' in the example. To view this tab, right-click on vessel procedure 'P-1' and select **Equipment Data** on the context menu of that procedure. By default, SuperPro Designer uses a built-in model to estimate purchase costs for each piece of equipment. However, you can override this estimate by either using your own model or specifying an exact purchase cost (from a vendor quote, for instance).

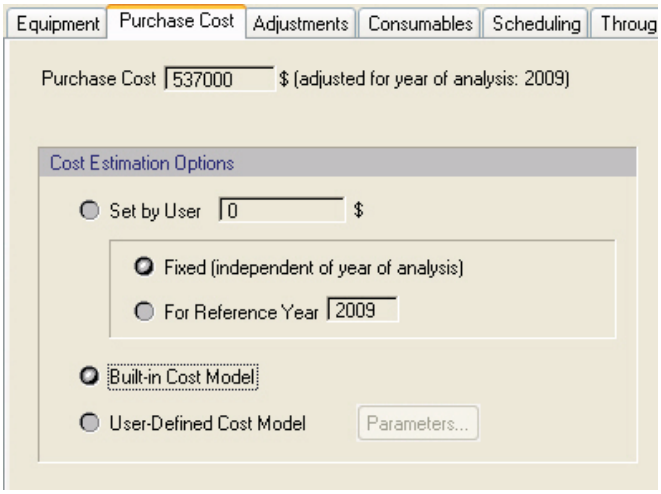


Figure 2.35: The 'Purchase Cost' tab of the 'Equipment Data' dialog.

Adjustments

Now please click on the 'Adjustments' tab of this dialog to view the number of standby units, the material, installation and maintenance cost factors, the percentage of purchase cost that is already depreciated, and the usage and availability rates for the batch reactor. The fields on this tab are described in detail below:

Number of Standby Units: For pieces of equipment that are critical to the operation of a process, you may choose to have one or more standby units (in case the regularly used pieces of equipment go down for scheduled or unscheduled maintenance). The number of standby units affects the capital investment but has no impact on maintenance and labor cost.

Material Factor: The purchase cost that is estimated using the built-in model corresponds to a certain material of construction that is displayed on this tab. Selecting a different material will affect the equipment purchase cost. The material cost factors for each type of equipment can be viewed by selecting **Equipment Materials** on the **Databanks** menu. Additional materials and material factors can be added to the 'User' database.

Installation Cost Factor: This factor is used to estimate the installation cost for each piece of equipment as a fraction of their purchase cost. The most common value is 0.3, meaning that the installation cost is 30% of the equipment purchase cost.

Maintenance Cost Factor: This factor is used to estimate the annual maintenance cost for each piece of equipment. The most common value is 0.1, meaning that the annual maintenance cost is 10% of its purchase cost.

Portion of Purchase Cost Already Depreciated: Oftentimes, a piece of equipment has already been either fully or partially depreciated. This can be captured using this variable. Any values other than 0.0% reduce the cost of depreciation but have no impact on the maintenance cost because that cost depends on the full purchase cost and not just the un-depreciated portion.

Usage and Availability Rates: These factors represent the equivalent of equipment rental rates. They are optionally used to estimate the Facility-Dependent (overhead) cost; for a description of this cost, see Chapter 9 (Economics).

If a piece of equipment is shared by multiple unit procedures, its purchase cost-dependent expenses (e.g., depreciation, maintenance, etc.) are distributed to its hosting steps based on the occupation time of each step.

Cost of Consumables

Consumables include materials and items that need to be replaced periodically, such us chromatography resins, cartridges of membrane filters, lubricants of equipment, etc. Disposable equipment, such as plastic bags, plastic bioreactors, roller bottles, etc. that are used once and thrown away belong to this category too. Parameters related to consumables are specified through the 'Consumables' tab of the 'Equipment Data' dialog. SuperPro Designer features a Consumables databank (as part of the 'User' database) where users can store information for all the consumables that they utilize. The information in the Consumables databank is accessible through the 'Consumables' tab of an equipment.

ECONOMIC PARAMETERS AT THE SECTION LEVEL

Division of a process into sections facilitates reporting of results for economic evaluation, raw material requirements, and throughput analysis of integrated processes. A process section is a group of unit procedures that have something in common. All processes initially contain one section (called the 'Main Section' by default). For information on how to create process sections and edit their properties, see 2.2b Specifying Process Sections.

Section-level Capital Investment Factors

SuperPro Designer uses a factor-based method to estimate the capital investment associated with each section of a process. These factors have been assigned default values that should be reasonable for most cases. However, you should still check these factors to ensure that they are accurate for your situation. You can then adjust the factors to better suit your particular process file. Figure 2.36 shows the 'DFC' tab of a section's 'Capital Cost Adjustments' dialog. This tab allows you to edit factors used to estimate the direct fixed capital (DFC) of a section. The 'Capital Cost Adjustments' dialog is brought up by selecting the appropriate section ('Main Section' in this case) in the relevant drop-down list box on the 'Section' toolbar, and then clicking on the **Capital Cost Adjustments** ( ) button on the same toolbar. Alternatively, you may click **Process Options ▸ Section: <section name> ▸ Capital Cost Adjustments** on the **Edit** menu, or you can right-click on the flowsheet to bring up its context

menu and then click **Section: <section name> ▸ Capital Cost Adjustments** (note that the term in brackets represents the name of the selected section).

The 'Distributed Set of PC-Factors' in the 'DFC' tab and the 'Startup and Validation Cost' factor in the 'Misc' tab can also be retrieved from a database site by allocating one or more process sections to that database site.That is the best way to utilize meaningful parameters for different industries around the globe. It is also the recommended way for standardizing cost analysis assumptions. For more information on how to take advantage of the database capabilities of SuperPro Designer for cost analysis, please consult the 'SynPharmDB' readme file in the 'Examples\SynPharm' directory of SuperPro Designer. Also, see 15.13 Sites & Resources Databank.

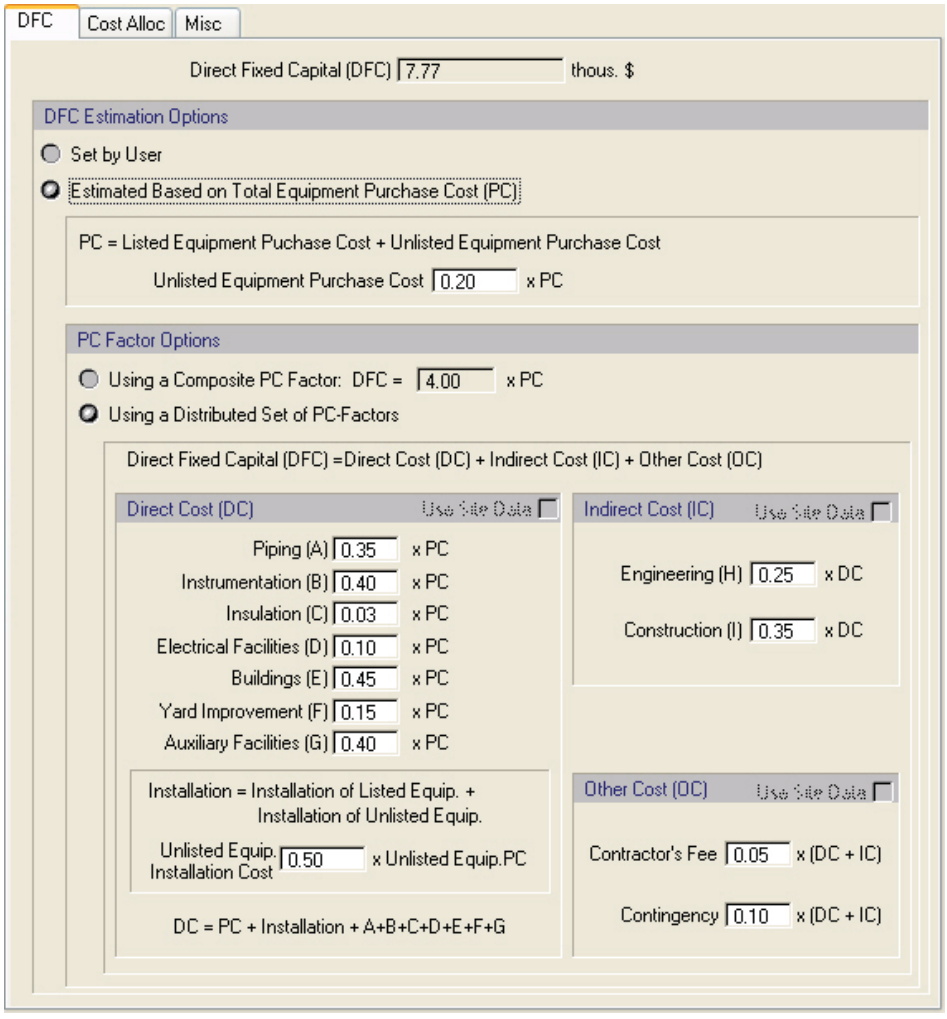

DFC
Cost Alloc
Misc
Direct Fixed Capital (DFC) 7.77 thous. $
DFC Estimation Options
Set by User
Estimated Based on Total Equipment Purchase Cost (PC)
PC = Listed Equipment Puchase Cost + Unlisted Equipment Purchase Cost
Unlisted Equipment Purchase Cost 0.20 x PC
PC Factor Options
Using a Composite PC Factor: DFC = 4.00 x PC
Using a Distributed Set of PC-Factors
Direct Fixed Capital (DFC) =Direct Cost (DC) + Indirect Cost (IC) + Other Cost (OC)
Direct Cost (DC)
Use Site Data
Piping (A) 0.35 x PC
Instrumentation (B) 0.40 x PC
Insulation (C) 0.03 x PC
Electrical Facilities (D) 0.10 x PC
Buildings (E) 0.45 x PC
Yard Improvement (F) 0.15 x PC
Auxiliary Facilities (G) 0.40 x PC
Installation = Installation of Listed Equip. + Installation of Unlisted Equip.
Unlisted Equip. Installation Cost 0.50 x Unlisted Equip.PC
DC = PC + Installation + A+B+C+D+E+F+G
Indirect Cost (IC)
Use Site Data
Engineering (H) 0.25 x DC
Construction (I) 0.35 x DC
Other Cost (OC)
Use Site Data
Contractor's Fee 0.05 x (DC + IC)
Contingency 0.10 x (DC + IC)

Figure 2.36: Adjusting the capital cost parameters at the section level.

Section-level Operating Cost Factors

SuperPro Designer calculates and reports nine cost items for each process section: Materials, Labor-Dependent, Facility-Dependent, Laboratory/QC/QA, Consumables, Waste Treatment/Disposal, Utilities, Transportation, and Miscellaneous Costs. Figure 2.37 displays the options available for calculating the facility-dependent operating cost.

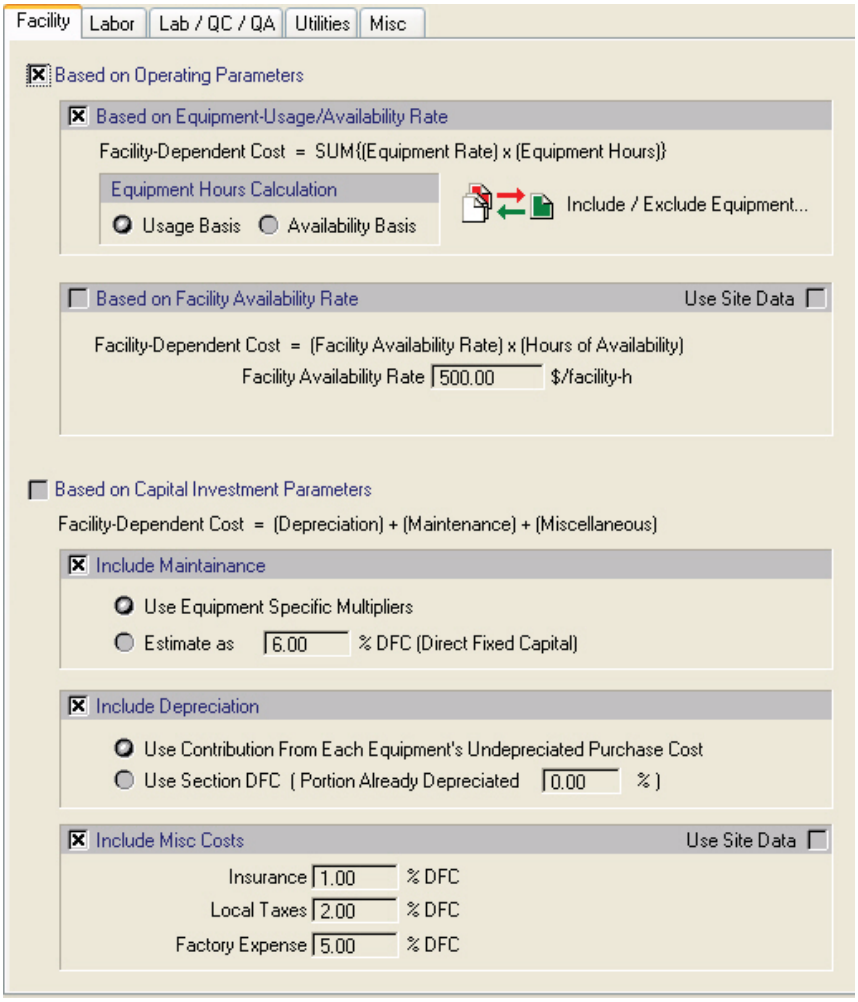

Facility
Labor
Lab / QC / QA
Utilities
Misc
Based on Operating Parameters
Based on Equipment-Usage/Availability Rate
Facility-Dependent Cost = SUM{(Equipment Rate) x (Equipment Hours)}
Equipment Hours Calculation
Usage Basis
Availability Basis
Include / Exclude Equipment...
Based on Facility Availability Rate
Use Site Data
Facility-Dependent Cost = (Facility Availability Rate) x (Hours of Availability)
Facility Availability Rate 500.00 $/facility-h
Based on Capital Investment Parameters
Facility-Dependent Cost = (Depreciation) + (Maintenance) + (Miscellaneous)
Include Maintainance
Use Equipment Specific Multipliers
Estimate as 6.00 % DFC (Direct Fixed Capital)
Include Depreciation
Use Contribution From Each Equipment's Undepreciated Purchase Cost
Use Section DFC (Portion Already Depreciated 0.00 %)
Include Misc Costs
Use Site Data
Insurance 1.00 % DFC
Local Taxes 2.00 % DFC
Factory Expense 5.00 % DFC

Figure 2.37: Adjusting the operating cost parameters at the section level.

This dialog is brought up by selecting the appropriate section ('Main Section' in this case) in the 'Section Names' drop-down list that is available on the **Section** toolbar and then clicking **Operating Cost Adjustments** ( ) on the same toolbar. Alternatively, you may select **Process Options ▸ Section: <section name> ▸ Operating Cost Adjustments** on the **Edit** menu, or you can right-click on the flowsheet to bring up its context menu and select **Section: <section name> ▸ Operating Cost Adjustments** (note that the term in brackets represents the name of the selected section). Through the 'Operating Cost Adjustments' interface, the user can adjust parameters that affect the Facility, Labor, Lab/QC/QA, Utilities,

and Miscellaneous costs of a section. In your example, please change the Facility Cost to be based on an Equipment Usage Rate. This will account for depreciation, maintenance, and miscellaneous equipment expenses. To do that, uncheck the default option entitled 'Based on Capital Investment Parameters' and check the option entitled 'Based on Operating Parameters', as shown in Figure 2.37. Also make sure that the 'Usage Basis' option is selected for the calculation of equipment hours. The equipment usage or availability rates are equipment-dependent, they are initialized to $100/h and they can be edited through the 'Adjustments' Tab of the Equipment Data dialog.

Next, please visit the other tabs on the above dialog to familiarize yourself with their functions. Notice that in the 'Labor' tab there are various options for specifying the labor costs of your process, including lumped and itemized estimates for the labor hours and labor cost rate. Furthermore, the 'Lab/QC/QA' tab allows you to specify information for a detailed calculation of laboratory, quality control and quality assurance expenses; for more details, see Chapter 9 (Economics). After you are done, click **OK** to apply the changes made to this dialog and return to the flowsheet.

ECONOMIC EVALUATION FACTORS AT THE PROCESS LEVEL

Finally, there are parameters at the process level that affect the results of project economic evaluation. These are specified through the 'Economic Evaluation Parameters for Entire Project' dialog. This dialog box is brought up by selecting **Process Options ▸ Economic Evaluation Parameters** on the **Edit** menu (or, you can right-click on the flowsheet to bring up its context menu and select **Economic Evaluation Parameters**).

In the 'Time Valuation' tab (see Figure 2.38) of this dialog, the user can specify various time

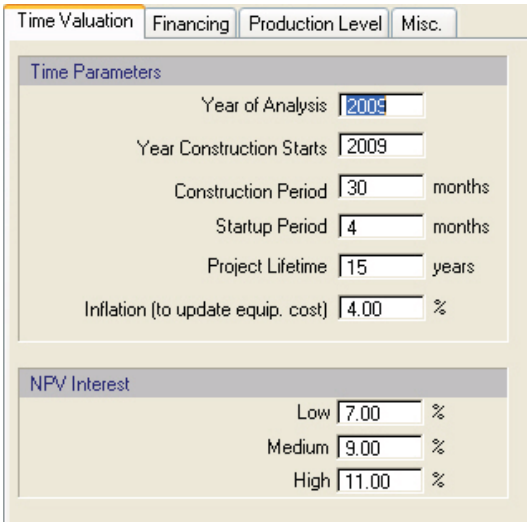


Figure 2.38: Adjusting the economic evaluation parameters at the process level.

parameters as well as the interest levels for calculating the net present value (NPV) of the project.

In the 'Financing' tab of the above dialog, the user can provide information on the financing of the project (e.g., equity versus borrowed money for DFC, working capital, etc.), the method of

depreciation, the depreciation period, the salvage value and the DFC outlay (the spending of direct fixed capital as a function of time).

In the 'Production Level' tab of the above dialog, the user can specify the capacity utilization profile (production level) for the expected lifetime of the project and provide information for product failure rate and disposal cost of scrapped product. Please note that the production level only affects the Cash Flow Analysis calculations. It has no impact on other project economic evaluation variables.

In the 'Miscellaneous' tab of the above dialog, the user can provide information for estimating income tax, advertising and selling expenses, and running royalties.

For the definitions of the different economic factors and for a description of how these are calculated, please consult Chapter 9 (Economics).

PERFORMING ECONOMIC CALCULATIONS AND VIEWING THE RESULTS

After simulating the process, you can carry out the economic calculations by clicking **Perform Economic Calculations** on the **Tasks** menu. The same can be accomplished by clicking **Perform Economic Calculations** ( ) on the **Main** toolbar or pressing **Shift+F9** (hold down the **Shift** key and hit the **F9** key on your keyboard). Depending on your interest, you may then do the following:

1. View the equipment purchase cost for each process step. To do that, right-click on a desired unit procedure icon, select **Equipment Data** on the context menu of that procedure, and in the 'Equipment Data' dialog that appears switch to the 'Purchase Cost' tab. Remember that the displayed purchase cost is for a single piece of equipment. If the requirements to carry out the specific processing task are such that more than one equipment item (of the same size) is needed, the total cost is the indicated cost times the number of equipment items. The number of equipment items is displayed on the first tab of the 'Equipment Data' dialog.
2. Select **Executive Summary** on the **View** menu to view summary economic analysis results for the entire project. Please view the contents of the 'Executive Summary' dialog for your example process now. The corresponding 'Summary' tab in that dialog should look similar to Figure 2.39 shown below.
3. To view the detailed results which were used to produce the Executive Summary, you will need to generate the *Economic Evaluation Report* (EER). To generate and view this report, select **Economic Evaluation (EER)** on the **Reports** menu. Any report can be created in different file formats. You can set the format and many other settings from the dialog that comes up if you select **Options** on the **Reports** menu. The EER contains an executive summary that presents the key analysis results, a breakdown of the total capital cost, a breakdown of the annual operating cost and a description of profitability analysis calculations. Please generate and view the Economic Evaluation Report now.
4. Another useful economic report is the *Itemized Cost Report* (ICR). This report contains detailed cost breakdowns of the total annual operating cost over all process sections. This includes all cost items that are calculated at the section level. Additional cost items that are calculated at the process level are not considered. To generate this report, select **Itemized Cost (ICR)** on the **Reports** menu.

5. Finally, a *Cash Flow Analysis Report (CFR)* can be generated. This report includes loan information and detailed breakdowns of capital outlay, loan payment and cash flow for each year over the expected lifetime of a project. To generate this report, select **Cash Flow Analysis (CFR)** on the **Reports** menu.

The equipment purchase cost shown in the 'Purchase Cost' tab of the 'Equipment Data' dialog corresponds to a single equipment unit.

For more information on the contents of the economic reports, please refer to the synthetic pharmaceutical example (see 2.2f Cost Analysis and Economic Evaluation), the β-Galactosidase example (see 2.3f Cost Analysis and Economic Evaluation) and the industrial wastewater treatment example (see 2.4c Cost Analysis and Economic Evaluation). For a detailed description of economic reports, see Chapter 12 (Reports).

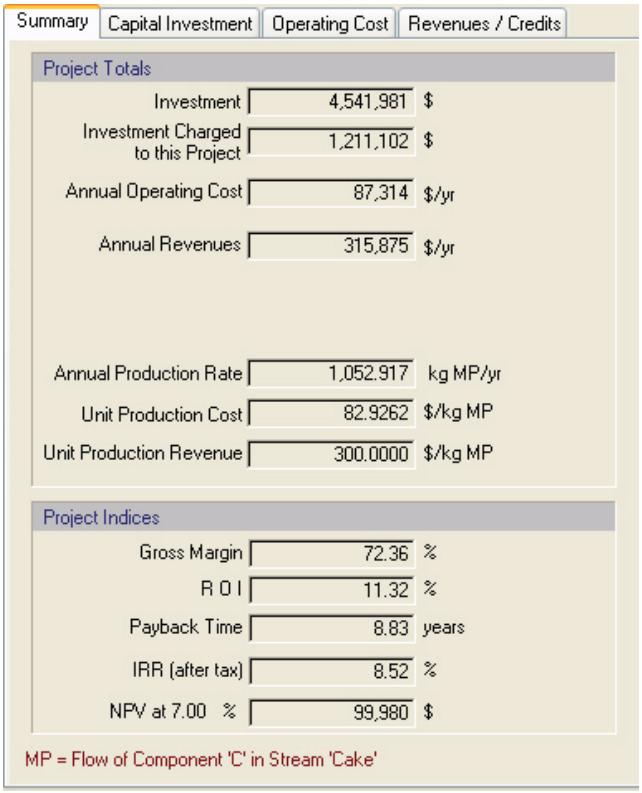

Summary
Capital Investment
Operating Cost
Revenues / Credits
Project Totals
Investment 4,541,981 $
Investment Charged to this Project 1,211,102 $
Annual Operating Cost 87,314 $/yr
Annual Revenues 315,875 $/yr
Annual Production Rate 1,052.917 kg MP/yr
Unit Production Cost 82.9262 $/kg MP
Unit Production Revenue 300.0000 $/kg MP
Project Indices
Gross Margin 72.36 %
R O I 11.32 %
Payback Time 8.83 years
IRR (after tax) 8.52 %
NPV at 7.00 % 99,980 $
MP = Flow of Component 'C' in Stream 'Cake'

Figure 2.39: The 'Summary' tab of the 'Executive Summary' dialog for the example process.

2.1n Environmental Impact

SuperPro Designer generates two different reports that provide information on the environmental impact of a process. The Emissions Report (select **Emissions (EMS)** on the **Reports** menu) provides information on all emitted components including volatile organic compounds (VOCs) and other regulated compounds. The Environmental Impact Report (select

Environmental Impact (EIR) on the **Reports** menu) provides information on the amount and type of waste generated by a manufacturing facility. It also provides information on the fate of a compound that enters an integrated manufacturing or waste treatment facility; for more details on these reports, see Chapter 12 (Reports).